

DFT OPTIMIZED STRUCTURES FOR CHAPTER 3: MULTIREFERENCE
GROUND AND EXCITED STATE ELECTRONIC STRUCTURES OF FREE- VER-
SUS IRON PORPHYRIN-CARBENES

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Free carbene/B3LYP/6-311G(d)/Triplet/0 degrees Constrained Optimization

C	0.00716416517195	-1.36512622960607	3.38804207482502
C	-1.40864546749185	-1.30218072809239	3.93806779486901
C	-0.00183490118175	0.98143083928367	-1.03846959200565
C	0.01295645692773	-0.09488545550133	-0.04504541478153
C	-0.01243531596127	-0.06570747370488	1.39031070520965
O	-0.05406730411541	0.97509092426193	2.02876086688951
O	0.01997024807571	-1.29946304258405	1.94171611137301
H	-2.03161296123600	-2.08429446749293	3.49679596032901
H	-1.39554839966549	-1.44736354314953	5.02270557519615
H	-1.86347472599478	-0.33182942056755	3.73125839691303
H	0.62245174183112	-0.55602629945797	3.78495464231999
H	0.48211286680434	-2.32073634839561	3.61326705882010
H	-0.89298449317386	0.92841894677856	-1.67698737372564
H	0.00588218390806	1.96149003213987	-0.54503801869703
H	0.86775668110148	0.92623621208827	-1.70506865453462

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Free carbene/B3LYP/6-311G(d)/Triplet/10 degrees Constrained Optimization

C	0.00012229988172	-1.41053824397258	3.36538311661752
C	-1.39164902814550	-1.25665257564127	3.95722168988733
C	0.13301880975582	0.97520912132511	-1.03583205268728
C	-0.04866587911647	-0.09321768688245	-0.05030524760823
C	0.01080577329313	-0.08382978154602	1.38488576125176
O	0.06809211360247	0.94791446380620	2.03626617282377
O	-0.02429007367236	-1.32445200221661	1.92017592287074
H	-2.08040876097772	-1.98618838221504	3.52373194842708
H	-1.35852512181780	-1.41911018725272	5.03898538144817
H	-1.78276735393837	-0.25374138643059	3.77692975195254
H	0.68215393940131	-0.65266564456168	3.75411040732794
H	0.41268258667281	-2.40037751768986	3.56400206080582
H	-0.55195795181720	0.86413872922759	-1.88361745568083
H	-0.03664074828611	1.95937557816391	-0.58025426494746
H	1.15222818416428	0.96731212888602	-1.44641305948887

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Free carbene/B3LYP/6-311G(d)/Triplet/20 degrees Constrained Optimization

C	-0.00186668399030	-1.42670218329072	3.36286516318896
C	-1.39075965042772	-1.25031442791093	3.95511844207266
C	0.28629101118865	0.93870957550754	-1.03815144343970
C	-0.05999872443629	-0.07552334531589	-0.03974611958931
C	0.03364948693294	-0.08086863643082	1.39477169986493
O	0.11473081317196	0.94224768620960	2.05642839074626
O	-0.02395154765606	-1.32576237501558	1.91821836024527
H	-2.09362904004817	-1.96214203817771	3.51491364492708
H	-1.36155067638478	-1.42279855264423	5.03545841672607
H	-1.76178327491573	-0.23826431684694	3.78355012595702
H	0.69531956338445	-0.68691932406360	3.7592650772326
H	0.39022867859822	-2.42674786163665	3.55147302259632
H	-0.37079398916350	0.88713831725408	-1.91299025722077
H	0.2159478772354	1.94933857024661	-0.61439566008179
H	1.31383507702279	0.79747855811522	-1.40150873071625

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Free carbene/B3LYP/6-311G(d)/Triplet/30 degrees Constrained Optimization

C	-0.00553883201289	-1.44085943232072	3.36269493076564
C	-1.39322051551747	-1.25026644030223	3.95324585837825
C	0.43607841078125	0.87502041058449	-1.04506862846965
C	-0.06080059473720	-0.05014692022982	-0.02455604185810
C	0.05432492386516	-0.07243417205533	1.41001254467157
O	0.15104798665765	0.93995400759130	2.08471583536583
O	-0.02269458493157	-1.32254728460123	1.91884428249610
H	-2.10543991463307	-1.94664969416986	3.50355169446433
H	-1.36945681601160	-1.43481627006287	5.03169544904504
H	-1.74870240315867	-0.23101699246804	3.79181826492015
H	0.70180842539857	-0.71660583347170	3.76932545690983
H	0.37081189364644	-2.44891071521469	3.54025659939924

H	-0.20646944112213	0.88326932165620	-1.93204520451658
H	0.49498313538461	1.90156899021211	-0.65814489017394
H	1.44101723239094	0.58308568185238	-1.38107601839771

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Free carbene/B3LYP/6-311G(d)/Triplet/40 degrees Constrained Optimization

C	-0.01154968136861	-1.45540057649185	3.36352835328709
C	-1.39834108912038	-1.25244733398953	3.95190842233552
C	0.57540107597556	0.78531791204125	-1.05592319576518
C	-0.05120262329102	-0.01823866858592	-0.00502676660230
C	0.07496445304880	-0.05916062729292	1.43037760554067
O	0.18460695022751	0.93983183303177	2.12118548609379
O	-0.02236894143351	-1.31548961137370	1.92107127347323
H	-2.11929223701270	-1.93142385141186	3.48971882361415
H	-1.38130352354815	-1.45280639720953	5.02765627272016
H	-1.73784227171454	-0.22573238165534	3.80401903638520
H	0.70524780025059	-0.74798387043923	3.78287502720905
H	0.34890990850713	-2.47158881544441	3.52708111591054
H	-0.05092262144574	0.83636910986685	-1.95302449994127
H	0.76488437782416	1.81431955064817	-0.71888960989991
H	1.53639559710090	0.34757678130626	-1.36128721136074

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Free carbene/B3LYP/6-311G(d)/Triplet/50 degrees Constrained Optimization

C	-0.02022710982939	-1.46901317666459	3.36469380047511
C	-1.40610939956186	-1.25566945147273	3.95144369421206
C	0.70104437604524	0.67157094331524	-1.06890151327975
C	-0.03014892429438	0.01598248223628	0.01568146044184
C	0.09365821438679	-0.04357041685267	1.45299828024590
O	0.21274188723431	0.94079467461469	2.16102484709673
O	-0.02432100440327	-1.30622367427416	1.92412664561978
H	-2.13491995654044	-1.91718520491295	3.47647574480444
H	-1.39565721656605	-1.47271499524786	5.02403714553289
H	-1.73053942546934	-0.22210388601169	3.81830167732745
H	0.70485194305126	-0.77826602415799	3.79727645834819
H	0.32537888051684	-2.49264422341188	3.51321474501603
H	0.09011803046747	0.75001116236204	-1.97464096395722
H	1.01878695599912	1.68763762601120	-0.79277024810761
H	1.59986993296372	0.09820687546706	-1.33769164177585

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Free carbene/B3LYP/6-311G(d)/Triplet/60 degrees Constrained Optimization

C	-0.03095330946564	-1.48168123945983	3.36767973991462
C	-1.41706274969521	-1.25670089722156	3.94933385563587
C	0.80822364543193	0.53655605164782	-1.08233205069800
C	0.00620516963578	0.04772405088166	0.03797556690598
C	0.11265707293268	-0.02927644807707	1.47713268332858
O	0.23569567031159	0.94101792832061	2.20201294548404
O	-0.02340639100182	-1.29805236457776	1.92912183477222
H	-2.15252773433920	-1.90003432413819	3.45985343873923
H	-1.41611949778624	-1.49090508566570	5.01836991366401
H	-1.72538008717010	-0.21653515041161	3.83062742107919
H	0.70164368662547	-0.80807342939878	3.81439004843539
H	0.29856758252772	-2.51244808059411	3.50295897097503
H	0.20497569233110	0.62896202819654	-1.99203682556311
H	1.24814281558993	1.52405458030269	-0.87744358947374
H	1.63007349807201	-0.15713863980471	-1.31237382119932

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Free carbene/B3LYP/6-311G(d)/Triplet/70 degrees Constrained Optimization

C	-0.04314097119297	-1.49093723999274	3.37163530836297
C	-1.43027856765564	-1.25722455643823	3.94715516466138
C	0.89356215775222	0.38370295262092	-1.09415908938310
C	0.05011672263565	0.07009996459950	0.05649378859503
C	0.12912131895778	-0.01896126134740	1.49743637598077
O	0.25480255488881	0.94047194102945	2.23453906251664
O	-0.02506005570761	-1.29194701965075	1.93487595527588
H	-2.16945453263472	-1.88837418124244	3.44750848588396

H	-1.43848226106915	-1.50058313926577	5.01409949836585
H	-1.72697991669177	-0.21288481797980	3.83569954942177
H	0.69367321364942	-0.82967537909797	3.82974408694945
H	0.27498145383835	-2.52643691993112	3.49804226027451
H	0.29307837684156	0.49723765123016	-2.00349077858029
H	1.45522215824334	1.32006897059174	-0.95603005002389
H	1.62057982114474	-0.41880358812555	-1.28827948630095

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Free carbene/B3LYP/6-311G(d)/Triplet/80 degrees Constrained Optimization

C	-0.05531464835317	-1.49815184410185	3.37497960070704
C	-1.44300877794583	-1.25736058219291	3.94611055589882
C	0.95266085641711	0.22089550840069	-1.10303992276272
C	0.09444055358204	0.08129880950676	0.06961043886050
C	0.13992347779265	-0.01395592424854	1.51104937077175
O	0.26711549550893	0.93829667764899	2.25594556978132
O	-0.02962214886755	-1.28955539416500	1.93953367420731
H	-2.18502713580424	-1.87940279590841	3.43931683580681
H	-1.45776648043392	-1.50734571659724	5.01146427361403
H	-1.73079634894271	-0.20999611831106	3.83992348366115
H	0.68444757483484	-0.84539203923190	3.84051285133305
H	0.25435120992142	-2.53690338585667	3.49592461509512
H	0.35514755321613	0.35562579977490	-2.01157518408397
H	1.62457350262872	1.08920952780608	-1.02624905762305
H	1.57575657844559	-0.67275612152382	-1.25823697326714

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Free carbene/B3LYP/6-311G(d)/Triplet/90 degrees Constrained Optimization

C	0.00367507025419	-1.37449399758513	3.44715837523878
C	-1.43479618482576	-1.33108047200902	3.93602227622560
C	0.97746383923203	0.00599818123970	-1.13082578122605
C	0.10358798989976	-0.03040766250810	0.03847860950232
C	0.05447266214168	-0.01578804020329	1.47908684654424
O	-0.02687718178937	0.99314059397706	2.15199221837209
O	0.07721974513321	-1.26922114202630	2.00221445977111
H	-2.03431723674797	-2.10349644739005	3.44792751327394
H	-1.46794033887145	-1.50455455926158	5.01604903484959
H	-1.88435182662844	-0.35727046329616	3.73504272618644
H	0.59764162446656	-0.57407891449860	3.89058172510936
H	0.47295594616529	-2.33454923898398	3.66534024759804
H	0.84559439714134	0.92168116386191	-1.72294820880924
H	2.03325548529511	-0.03435678625396	-0.82674556792411
H	0.80203352613382	-0.84344868106250	-1.80410434271212

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Free carbene/B3LYP/6-311G(d)/Triplet/100 degrees Constrained Optimization

C	0.04175291094307	-1.26209748183926	3.46937794269639
C	-1.39299149525595	-1.38349562742160	3.95580036087496
C	0.98442525833194	-0.20649536848510	-1.11959318334955
C	0.02804897067739	-0.13080280029419	-0.01948149981558
C	-0.06732594804615	-0.03419356611847	1.41820186833560
O	-0.28442695751942	0.99723885389313	2.02177607892360
O	0.10997356645880	-1.23938583367639	2.02047891087996
H	-1.87822208225625	-2.26039723489281	3.51986450279124
H	-1.41125854630466	-1.48902353610340	5.04497311246450
H	-1.96922738399232	-0.49510732953228	3.69165170112654
H	0.51807751291926	-0.36149985163787	3.85966223808433
H	0.63563738690603	-2.13341533117330	3.74839092529711
H	1.59286754101300	0.70705223534184	-1.19452511710489
H	1.67156470934282	-1.05977092488170	-1.01232411914859
H	0.46884473978243	-0.32704068317861	-2.07898359005563

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Free carbene/B3LYP/6-311G(d)/Triplet/110 degrees Constrained Optimization

C	0.03994300823117	-1.27492585375744	3.44411102203850
C	-1.38154928610807	-1.37166708550604	3.97305042877940
C	0.94085937193513	-0.37599137865922	-1.10914654669175
C	-0.01469945296498	-0.11799809956721	-0.03514702725525

C	-0.09960142693876	-0.02982346798802	1.40361448225872
O	-0.27633949282921	1.00272129413982	2.01763269662418
O	0.06447110110968	-1.24420174858304	1.99421631775877
H	-1.89672647831164	-2.23643065085255	3.54725038709370
H	-1.36923039770937	-1.48323822061466	5.06172906155817
H	-1.94798088393231	-0.47072439053182	3.73094381455598
H	0.54484893841019	-0.38578090019317	3.82480360424996
H	0.62518472092446	-2.15901874797239	3.70064354138438
H	1.67283859774649	0.43979224653035	-1.20118743908042
H	1.49824993259314	-1.31186620934691	-0.95079403549460
H	0.43316496484406	-0.46075139809769	-2.07645017577975

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Free carbene/B3LYP/6-311G(d)/Triplet/120 degrees Constrained Optimization

C	0.03861089065237	-1.28955205340484	3.41699936682810
C	-1.36953422034218	-1.36239590499294	3.98408855451376
C	0.86543020932521	-0.53419545449362	-1.09499917797236
C	-0.05234656522789	-0.09428983761948	-0.04609929647117
C	-0.12598138886895	-0.01894716977883	1.39294694007170
O	-0.26487925031813	1.01090539017786	2.02096071890895
O	0.02410616626978	-1.24447887904325	1.96766638794765
H	-1.91414461361190	-2.21204120806239	3.56450901030826
H	-1.32977967466003	-1.48503157995696	5.07092170535959
H	-1.92319139298220	-0.44749230001622	3.76602397410805
H	0.57170829157084	-0.41451170668037	3.79198066145613
H	0.61236075442844	-2.18785324583156	3.64920014260454
H	1.70997630991527	0.16192360170454	-1.20168790370472
H	1.27661936905876	-1.53384052201605	-0.88907772063787
H	0.36425334279060	-0.58018372598589	-2.06816323132062

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Free carbene/B3LYP/6-311G(d)/Triplet/130 degrees Constrained Optimization

C	0.03704563169305	-1.30534679097708	3.39601943375438
C	-1.36183703643322	-1.35640315437640	3.98794262556517
C	0.76188371670862	-0.67318612571154	-1.08363341236126
C	-0.07464902262604	-0.06769528879439	-0.04839161157938
C	-0.13757870255506	-0.00722357338911	1.38981757608112
O	-0.24744470620689	1.01757462173130	2.03236537024361
O	-0.00197066195666	-1.24383766277265	1.94806865065932
H	-1.93117541680744	-2.18988180715979	3.56873804205355
H	-1.30485813144425	-1.49269841333569	5.07239111060267
H	-1.90028917564493	-0.42789246253000	3.79048073435450
H	0.59397274253578	-0.44506160546745	3.77055054571898
H	0.59678976581892	-2.21733995325458	3.60836407816484
H	1.69513462067886	-0.10754072821171	-1.21725908421734
H	1.02928461316668	-1.71091238077090	-0.83623725336917
H	0.25339838707257	-0.68437753898002	-2.05394667367097

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Free carbene/B3LYP/6-311G(d)/Triplet/140 degrees Constrained Optimization

C	0.03617329058358	-1.31893551086660	3.38256575422754
C	-1.35832422968765	-1.35384326631301	3.98596047565987
C	0.63394578118658	-0.79034164887414	-1.07571167594620
C	-0.08668806560130	-0.04353872520401	-0.04492758122704
C	-0.13702970307001	0.00329279580051	1.39211083681955
O	-0.22719684600489	1.02263047753295	2.04722352803955
O	-0.01302972345766	-1.24263151529733	1.93594574580791
H	-1.94481749432745	-2.17296482345366	3.56205960832748
H	-1.29415246679830	-1.50424861476015	5.06815297578500
H	-1.88307750735179	-0.41442204272046	3.80415922364618
H	0.60975054921697	-0.47122677021656	3.76063526055107
H	0.58313022796835	-2.24164059263747	3.58168996295784
H	1.63567274340273	-0.36823327442351	-1.23944539328551
H	0.75542475811754	-1.84676110404444	-0.79713804325768
H	0.11159496582330	-0.75589825952212	-2.03801054610557

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Free carbene/B3LYP/6-311G(d)/Triplet/150 degrees Constrained Optimization

C	0.03451292490658	-1.33034174640225	3.37546490585006
C	-1.35933739736519	-1.35516254696481	3.98093630329830
C	0.48674548227482	-0.88300381008131	-1.07164322663500
C	-0.08810322040394	-0.02238052955971	-0.03763047434596
C	-0.12526314294028	0.01324684733285	1.39825887960153
O	-0.19988980408775	1.02784900644693	2.06351160506585
O	-0.01584314748979	-1.24050773742835	1.93001069861110
H	-1.95532713370560	-2.16482316615115	3.55208863138434
H	-1.29515753341927	-1.51402035894455	5.06192316541992
H	-1.87422368302381	-0.40881533087933	3.80690260290565
H	0.61759250367157	-0.49209509432991	3.75999454826248
H	0.57187709090453	-2.26055010779049	3.56572030565112
H	1.53334073472040	-0.61297338877701	-1.27152370884175
H	0.46476604574341	-1.93896113188509	-0.76858230852002
H	-0.05365716878568	-0.79243165958581	-2.02016179570763

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Free carbene/B3LYP/6-311G(d)/Triplet/160 degrees Constrained Optimization

C	0.03401111280082	-1.33836301153173	3.37331508995971
C	-1.36229573001858	-1.35813120645280	3.97334730329095
C	0.32441790701222	-0.94945005929867	-1.06939356482568
C	-0.08699867577779	-0.00642096086682	-0.02913665586744
C	-0.10911699245035	0.02079390366595	1.40577010134105
O	-0.17503882616074	1.03176082752898	2.07825616938546
O	-0.00962935274657	-1.23832189648050	1.92861015251371
H	-1.96186820407256	-2.16135811535011	3.53735793262145
H	-1.30327698351156	-1.52415131903294	5.05355350963034
H	-1.87064420432229	-0.40750229892982	3.80339630449017
H	0.62094882025239	-0.50652730944328	3.76577931911631
H	0.56467170267260	-2.27322483443048	3.55961147718630
H	1.39383913068969	-0.84233013324008	-1.29968732968165
H	0.15389429883476	-1.98700385765632	-0.75138548457238
H	-0.22259705520205	-0.78574689248137	-2.00412419258831

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Free carbene/B3LYP/6-311G(d)/Triplet/170 degrees Constrained Optimization

C	-0.00056897165962	-1.37955323869807	3.37558028268190
C	-1.40510627547517	-1.33047164929714	3.95439456196820
C	0.18156238972744	-0.97906634582627	-1.06838553647573
C	-0.01487219599690	0.00801826535134	-0.00659860962778
C	-0.03741369705799	0.01272352908080	1.42744600141463
O	-0.05442315884850	1.01633840467784	2.11486104285439
O	-0.01499417938859	-1.25764310437194	1.93247613495532
H	-2.04061577508196	-2.09475065386959	3.49952617190633
H	-1.37223545993436	-1.51203195784172	5.03323740453888
H	-1.85877408896042	-0.35170050392095	3.78905114821683
H	0.62490971249975	-0.58682330840519	3.78909412495951
H	0.47508497524294	-2.34457274133818	3.55698638349550
H	1.08497797634391	-0.76476304432025	-1.65378082134051
H	0.28012917813380	-1.98698450760840	-0.64439269635625
H	-0.65859045854433	-0.98983609661229	-1.77422546119122

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Free carbene/B3LYP/6-311G(d)/Triplet/180 degrees Constrained Optimization

C	-0.00089783836368	-1.38007577933072	3.37971441237754
C	-1.41072512873764	-1.32997599795548	3.94556924017973
C	0.00565541644039	-0.99427109781086	-1.06663465208167
C	-0.01143876606290	0.00874500367909	-0.00179128736630
C	-0.01842083219133	0.01276064787758	1.43175910645727
O	-0.03369641216495	1.01616245591397	2.11968333978877
O	-0.00184644755948	-1.25828571592846	1.93645211802721
H	-2.04241884608757	-2.09465027403377	3.48612211006016
H	-1.38775491931005	-1.50995404167316	5.02490315407951
H	-1.86246478799609	-0.35123412735952	3.77485624996671
H	0.62103943331164	-0.58754975139933	3.79861810649377
H	0.47249268373305	-2.34532285220790	3.56547230769293
H	0.91505643683011	-0.92001009029879	-1.67685991481309
H	-0.03700854236142	-2.00632985119275	-0.64341702950768

H -0.84493434448007 -0.87386173627990 -1.74917712935486

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Free carbene/B3LYP/6-311G(d)/Triplet/190 degrees Constrained Optimization

C 0.02105807612112 -1.35692551080993 3.39810252998977
C -1.41098235101556 -1.35452780358742 3.90749095184903
C -0.02615774699481 -0.99711523244557 -1.05277474176412
C 0.06440073150316 0.00745235022880 0.00688103175137
C 0.02891142958907 0.02262734751786 1.44027217106312
O -0.04546361822706 1.02920928393306 2.11907278782363
O 0.07339195129695 -1.24363532158844 1.95497916349315
H -1.99608749129494 -2.14453811492808 3.42956506011671
H -1.42436911703643 -1.52690775952096 4.98820819898000
H -1.89056156195748 -0.39387982009571 3.71173654607914
H 0.59713643243393 -0.54003057660453 3.83522486507073
H 0.52093406872149 -2.30339399873701 3.60916959899891
H 0.89141333862738 -1.03839093744892 -1.65409380068875
H -0.19156923373030 -1.99422703058327 -0.62410106562460
H -0.84941780303650 -0.77957008332987 -1.74446316513807

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Free carbene/B3LYP/6-311G(d)/Triplet/200 degrees Constrained Optimization

C 0.00431720390873 -1.36064825096199 3.42099099507370
C -1.45059828530333 -1.33224195837099 3.86004441591476
C -0.02375044259791 -1.00469935402707 -1.03761524968069
C 0.21210959836496 -0.02561189627816 0.02372565295014
C 0.12753434144493 0.00373144755919 1.45618397083837
O 0.04072877746167 1.01649999709615 2.12358789780517
O 0.12856457488087 -1.25859273352135 1.98129933428811
H -2.02409526644332 -2.11677098615744 3.35954815090015
H -1.51911641081070 -1.49605623576790 4.93997944596107
H -1.90498923596255 -0.36581378632802 3.63470419327825
H 0.57168783056441 -0.54994215156967 3.88040790566556
H 0.47794542514987 -2.31340977225144 3.66201198583733
H 0.61873799490155 -0.82321469422158 -1.90628614708810
H 0.16636553753978 -2.02579652730157 -0.68028995229286
H -1.06280453809895 -0.96128630589813 -1.39302246745097

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Free carbene/B3LYP/6-311G(d)/Triplet/210 degrees Constrained Optimization

C 0.01884218085499 -1.33738879769556 3.44817250201557
C -1.45121938315989 -1.34950465537070 3.83427952006201
C -0.04990976768290 -1.00509609814294 -1.03608039517197
C 0.28964196301202 -0.06317679189657 0.03055527173014
C 0.17255129706000 -0.00734191711435 1.46157236686396
O 0.03728663472409 1.01509575308326 2.10487632961129
O 0.19174486733886 -1.25795336153383 2.01183457616494
H -1.98007773315371 -2.16227235703429 3.32968395391130
H -1.55372743454295 -1.49486196468978 4.91414734967256
H -1.92884970511653 -0.40337858782005 3.57340104941254
H 0.54254517691424 -0.49994402625728 3.91130839779025
H 0.51418543552895 -2.26926853361775 3.72449883546743
H 0.58852246190104 -0.86741588630089 -1.91565446585011
H 0.05926394376271 -2.04496013258888 -0.69829589203816
H -1.08816283244092 -0.86638585102040 -1.36902926764176

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Free carbene/B3LYP/6-311G(d)/Triplet/220 degrees Constrained Optimization

C 0.03220918022732 -1.31591916823384 3.47832993055281
C -1.44760641015707 -1.36591649163027 3.82160609004650
C -0.07375278158994 -0.99944174519386 -1.04571625692020
C 0.35594995230817 -0.11468251086549 0.03671959693864
C 0.20567614549765 -0.02896091312520 1.46506681609893
O 0.02445269085335 1.00370671757261 2.07909348236335
O 0.24523163186816 -1.26382875290832 2.04577871734160
H -1.93561539592678 -2.20638295365441 3.32125790807094
H -1.57781369272519 -1.48988143837605 4.90113215349488
H -1.94658013925259 -0.44164102884144 3.52468889674017

H	0.51587083756956	-0.45205785426939	3.93634193571758
H	0.54764502634509	-2.22520179067963	3.79069869861944
H	0.57252826824448	-0.90327867128207	-1.92510675175561
H	-0.06020727520109	-2.05339545635409	-0.73357551566637
H	-1.09535093306112	-0.75697115015853	-1.37104556964266

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Free carbene/B3LYP/6-311G(d)/Triplet/230 degrees Constrained Optimization

C	0.04436990202180	-1.29902801536396	3.50920120444733
C	-1.44051742080183	-1.37918529435416	3.82336359533905
C	-0.09344271669661	-0.98707188459757	-1.06627573792328
C	0.40959097424208	-0.17725468579839	0.04221874830803
C	0.22433802891676	-0.06069500339061	1.46651232242365
O	0.00078422792510	0.98115481765816	2.04927120780255
O	0.28622986685299	-1.27714037470204	2.07980745466020
H	-1.89616637590022	-2.24401519208198	3.33410772771529
H	-1.59023516700059	-1.48065707197631	4.90271659388877
H	-1.95674129101950	-0.47569930244861	3.49378521781355
H	0.49629570655080	-0.41172827703693	3.95463771582201
H	0.57633235355740	-2.18661139732356	3.85437723261409
H	0.56329464282869	-0.92103427355033	-1.94078411088056
H	-0.17319075972036	-2.04899561841596	-0.79108707844961
H	-1.08830486675651	-0.64589163461775	-1.38658196158106

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Free carbene/B3LYP/6-311G(d)/Triplet/240 degrees Constrained Optimization

C	0.05539436146740	-1.28693349907734	3.54145087759839
C	-1.43061411449214	-1.39072255262211	3.84303717731672
C	-0.10953191439637	-0.96610118354357	-1.10144333389805
C	0.44636554410189	-0.25358990018510	0.04692810345318
C	0.22878756906510	-0.10548891402547	1.46550573108955
O	-0.02631187638982	0.94667086304263	2.01515021519286
O	0.31180321516078	-1.30024417034607	2.11412612309474
H	-1.86228064032863	-2.27834506955739	3.37327807745670
H	-1.58933314768136	-1.46608649819075	4.92322283388841
H	-1.96276706950579	-0.50806120235944	3.48373573553150
H	0.48349537203463	-0.37781320644942	3.96593091839817
H	0.60260243143428	-2.15275643851797	3.91663641601078
H	0.56376056540901	-0.91491712521192	-1.96430716576789
H	-0.28070407647685	-2.03057371240075	-0.88127336916353
H	-1.06802911440212	-0.52889059855534	-1.41670820820151

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Free carbene/B3LYP/6-311G(d)/Triplet/250 degrees Constrained Optimization

C	0.05945224753695	-1.27071288374648	3.57535373459697
C	-1.42467031788551	-1.40136239165040	3.87586086399887
C	-0.10790407224032	-0.94518584630305	-1.14701680909055
C	0.46573427010178	-0.34032600374334	0.05193986903082
C	0.21295506080951	-0.15770795304787	1.46120339479570
O	-0.07065586819355	0.90566740994350	1.97455670650561
O	0.32114187325426	-1.32624647220373	2.14986172161892
H	-1.83233742820228	-2.31426172895104	3.43398013796927
H	-1.58552293215985	-1.44531727786212	4.95744869974537
H	-1.97718805556460	-0.54445124173765	3.48621932431557
H	0.46331900310375	-0.33737004919530	3.97000788581155
H	0.62647457368996	-2.10948397501892	3.98126691947340
H	0.60430508236854	-0.92015299842789	-1.97941031080251
H	-0.38391722407280	-1.99859844763911	-0.98669374594500
H	-1.00854910754583	-0.40834334841660	-1.47930826002397

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Free carbene/B3LYP/6-311G(d)/Triplet/260 degrees Constrained Optimization

C	0.06302008308382	-1.25731188893599	3.60334222616531
C	-1.41681681050470	-1.41095652388549	3.91401147032727
C	-0.10229341516018	-0.92118963322463	-1.19191745563843
C	0.47067829397126	-0.42597720860620	0.05552394175430
C	0.18602744629587	-0.21189176304636	1.45418008590373
O	-0.12241097449283	0.86044022469498	1.93444280477847

O	0.32071464508960	-1.35388857106282	2.17927779782306
H	-1.80559893746027	-2.34601379345688	3.50251439744747
H	-1.57285254189659	-1.42455346806332	4.99710911829673
H	-1.98947847657721	-0.57911143792415	3.49993923451556
H	0.44722563201891	-0.30278647255065	3.96574552341392
H	0.64990115559513	-2.06965158407248	4.03398973251450
H	0.64556944156737	-0.91967391212969	-1.99296364649742
H	-0.46997763727058	-1.95429987403464	-1.09559539914352
H	-0.94107079925959	-0.29698730170170	-1.53432969966094

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Free carbene/B3LYP/6-311G(d)/Triplet/270 degrees Constrained Optimization

C	0.06612300513978	-1.24656542034892	3.62448730286090
C	-1.40936899574014	-1.41816775419321	3.94605546020890
C	-0.09593425621739	-0.89658698807967	-1.22605643537782
C	0.48071667125482	-0.50788910831082	0.05705526025997
C	0.16072940624923	-0.26743457571494	1.44488676291603
O	-0.17483020706766	0.81149172901448	1.89240392674432
O	0.32104244691051	-1.38180715815832	2.20313950763444
H	-1.78202580191040	-2.37221020380685	3.56435916291205
H	-1.56105403150219	-1.40212755987465	5.02970589259344
H	-1.99864383419700	-0.60974301241314	3.50963264023270
H	0.43383784786511	-0.27443036591572	3.95613007345910
H	0.66952357640945	-2.03457625041166	4.07689529808058
H	0.66694823451434	-0.89655425269976	-2.01267899677390
H	-0.52360396964309	-1.91018057315996	-1.19260559001542
H	-0.89082298706536	-0.20707171392689	-1.54814013373528

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Free carbene/B3LYP/6-311G(d)/Triplet/280 degrees Constrained Optimization

C	0.07072102465719	-1.23362660895885	3.64081497666644
C	-1.39961379820599	-1.43142757771955	3.97067228700991
C	-0.09199990016769	-0.86865808841437	-1.24939051431811
C	0.49319809484025	-0.58603557546371	0.05787553685878
C	0.13739963401580	-0.32080643354742	1.43322529501707
O	-0.23213504105446	0.76076281168222	1.84776676283757
O	0.32730908605469	-1.40587548270604	2.22382689417305
H	-1.74941563598546	-2.40513634819778	3.61815934159634
H	-1.54977996289588	-1.38711126722785	5.05373973162002
H	-2.00896096187260	-0.65081503465139	3.51186434827389
H	0.41485451779071	-0.24305557102858	3.94204609410898
H	0.69390184754983	-1.99252049994517	4.11556975074999
H	0.67990906204630	-0.89121353326349	-2.02671962752245
H	-0.59208225168819	-1.84871250272754	-1.26547073372267
H	-0.83066861008450	-0.10962149583049	-1.54871001134879

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Free carbene/B3LYP/6-311G(d)/Triplet/290 degrees Constrained Optimization

C	0.07577654524856	-1.21853821902102	3.65445763047341
C	-1.38855217300530	-1.44815142593080	3.99045605108582
C	-0.09018990994023	-0.83802058867794	-1.26530360763993
C	0.50601146706919	-0.66824683958065	0.05742775245704
C	0.11774031916304	-0.37799501776874	1.41919510117163
O	-0.28843040507412	0.70478983087365	1.79682175091009
O	0.33894541299492	-1.42940734852616	2.24414641963119
H	-1.70979708469508	-2.44205769399006	3.66852135952038
H	-1.54075675802259	-1.37421940965375	5.07161066238426
H	-2.01964119165659	-0.70017661207221	3.50736882012787
H	0.39073615957873	-0.20915938900088	3.92370226416056
H	0.72011704675814	-1.94319873725363	4.15377652670545
H	0.68148423092166	-0.88074099691964	-2.04179994892290
H	-0.66099305056401	-1.77622286087245	-1.32910893670325
H	-0.76981350377631	-0.01250789960575	-1.52600171336160

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Free carbene/B3LYP/6-311G(d)/Triplet/300 degrees Constrained Optimization

C	0.08028375961690	-1.20228539224251	3.66507066885498
C	-1.37641680771683	-1.46721860255920	4.00828045781416

C	-0.09024423140631	-0.80488760792968	-1.27581889424040
C	0.51345215104433	-0.75679539674833	0.05484486890845
C	0.10190572955439	-0.43873613834242	1.40308104314418
O	-0.33850201343315	0.64493143110965	1.74059988837759
O	0.35177846488927	-1.45349593958103	2.26330594030766
H	-1.66506752595829	-2.48132348308866	3.72026310183889
H	-1.53238870032794	-1.36147570471246	5.08625921864365
H	-2.03052667928239	-0.75685302083643	3.49967719718462
H	0.36227122566787	-0.17459023570254	3.89952595855501
H	0.74675722532749	-1.88816893648875	4.18947827228421
H	0.67552025671833	-0.85165204469779	-2.05772934792970
H	-0.72073004398943	-1.69854417274542	-1.39152569660859
H	-0.71545570570423	0.07724203656555	-1.48004254513472

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Free carbene/B3LYP/6-311G(d)/Triplet/310 degrees Constrained Optimization

C	0.07929839086263	-1.18226616001954	3.67385433546598
C	-1.36991748949494	-1.47464113749819	4.02661000244908
C	-0.08198274089725	-0.78153656006625	-1.28413340814142
C	0.51173972856798	-0.85829036904146	0.05105978788020
C	0.08734420679635	-0.50560386492109	1.38537208801409
O	-0.38116942134970	0.58048416511210	1.67823410147037
O	0.35908074000962	-1.48026280808547	2.28337611191843
H	-1.62959730979029	-2.50668651131898	3.77737651123027
H	-1.53009977589146	-1.33241411720120	5.09977559204819
H	-2.04315986872330	-0.80298921024808	3.49102867889231
H	0.33168570031539	-0.13867692316288	3.86852812002126
H	0.76392911205172	-1.82813035452594	4.22499820201358
H	0.67967861731702	-0.86367612804066	-2.06680893980044
H	-0.79422537834264	-1.60404404180380	-1.44307387630459
H	-0.61996740643113	0.16488081282143	-1.44092717515733

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Free carbene/B3LYP/6-311G(d)/Triplet/320 degrees Constrained Optimization

C	0.08011021677258	-1.16901434615536	3.67839556842995
C	-1.36256967641042	-1.47168638412286	4.04868378647414
C	-0.07422386474789	-0.76143137383546	-1.29289536079202
C	0.48505961426824	-0.96066633607930	0.04511540820635
C	0.06618420815084	-0.57385220406532	1.36851792469900
O	-0.42296108191429	0.51412831346226	1.62309664981594
O	0.35843673044886	-1.51107112876021	2.29810415155389
H	-1.60688085505829	-2.51571555660716	3.83673763417177
H	-1.51987487474499	-1.29475834245121	5.11711730803788
H	-2.04887053621425	-0.82974216735131	3.49361766274836
H	0.31693194747428	-0.11542531292339	3.83528022812553
H	0.77749665373276	-1.78430876733707	4.24817272177749
H	0.69902607657987	-0.81992832865994	-2.06637189807616
H	-0.81778865470045	-1.53708210885069	-1.52481627932621
H	-0.56743879863684	0.21670083573700	-1.38348537384592

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Free carbene/B3LYP/6-311G(d)/Triplet/330 degrees Constrained Optimization

C	0.08174256287938	-1.15316101209432	3.68005830025074
C	-1.35146387186901	-1.47675964162046	4.06927181036723
C	-0.06576226838734	-0.74143543194699	-1.30009727152234
C	0.44246501895378	-1.05006047848590	0.03810717811348
C	0.03841276305944	-0.63036954842924	1.35381063051108
O	-0.47563854576259	0.45411859590925	1.57638327735751
O	0.35934781906619	-1.53092934209801	2.30948535418134
H	-1.57331260190202	-2.53195107552731	3.89055078546133
H	-1.50612226790471	-1.27112214961833	5.13295038871956
H	-2.05561487637959	-0.86761869070735	3.49979240093170
H	0.29554265562331	-0.09022962892355	3.80367694471954
H	0.79629086420117	-1.73473859710823	4.26381151074229
H	0.71949508681502	-0.81871838920838	-2.05965594296270
H	-0.85967608245045	-1.44473687626147	-1.58846020223988
H	-0.48306915094258	0.27385905812028	-1.34441503263088

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Free carbene/B3LYP/6-311G(d)/Triplet/340 degrees Constrained Optimization

C	0.08346483077704	-1.13651932696666	3.67940995372571
C	-1.33794998371547	-1.48719476065399	4.08819688566893
C	-0.05731335140678	-0.72322974690904	-1.30607380631965
C	0.38519961608806	-1.12632261762199	0.03067985676425
C	0.00655854715523	-0.67491751742295	1.34164497972467
O	-0.53255982966571	0.40286841757976	1.53948048611357
O	0.36031724056929	-1.54125936531291	2.31676206676583
H	-1.53348075465120	-2.55195675054534	3.93789488612179
H	-1.49008453558609	-1.25860779184841	5.14755330893864
H	-2.06207863225625	-0.91127476903182	3.50926370901550
H	0.27052380569733	-0.06571979406689	3.77517546102949
H	0.81718174833798	-1.68454397144496	4.27174779601737
H	0.74006063063833	-0.83626383357688	-2.04826265390310
H	-0.89949746905833	-1.34286399122706	-1.64474600931028
H	-0.38770475792342	0.32395261104912	-1.31345678835272

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Free carbene/B3LYP/6-311G(d)/Triplet/350 degrees Constrained Optimization

C	0.07504308254773	-1.09146852499211	3.68040843382211
C	-1.31565242091940	-1.54032103559418	4.09927925762182
C	-0.03428545771252	-0.70093850637019	-1.30793431622152
C	0.34426956884791	-1.16686837921971	0.02870654661077
C	-0.03575423868683	-0.69728275580406	1.33217406220131
O	-0.65027410339516	0.34473922279195	1.50091340817676
O	0.38335900017413	-1.50854183403986	2.32853194475356
H	-1.42783354473230	-2.62064995764005	3.97741510018523
H	-1.48673417780743	-1.29598597842252	5.15223348205066
H	-2.08177611028405	-1.03814451568783	3.50580940950026
H	0.17876022259337	-0.00738849312758	3.74944232844509
H	0.84809029425387	-1.56563407804117	4.28630217847527
H	0.65290483171355	-1.07285270517002	-2.07388496294388
H	-1.04214273941579	-1.04882757153226	-1.57648942148740
H	-0.04533710217710	0.39631190484958	-1.35763731919006

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Free carbene/B3LYP/6-311G(d)/RKS/10 degrees Constrained Optimization

C	-0.42226234927042	-0.78795868376621	3.52763948357066
C	-1.87847806158992	-0.63915609070724	3.93788360554309
C	0.27488727976639	1.17941943817564	-0.81143532515882
C	-0.04998785326365	-0.04573331402048	-0.09542296453240
C	-0.23159163362046	0.26231191219063	1.39672498626061
O	-0.29541775916847	1.36125803011021	1.90849191725662
O	-0.29038641609300	-0.88736217656610	2.08688774103026
H	-2.48003797373169	-1.45777462797763	3.53571948975236
H	-1.96038184223680	-0.65836855018047	5.02873061601250
H	-2.28924277942090	0.30787638809342	3.58379918465129
H	0.17713480041486	0.05405732387384	3.87812817593529
H	0.00608906062916	-1.72004533755486	3.89676931113251
H	1.38787969463557	1.08774563885221	-0.78947747372452
H	0.02771709846099	1.14253650110059	-1.87508922317173
H	0.03843109648836	2.14153702137645	-0.33963655355773

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Free carbene/B3LYP/6-311G(d)/RKS/20 degrees Constrained Optimization

C	-0.42218566903321	-0.78140817104953	3.51017704217227
C	-1.87325457851153	-0.64063520518159	3.94042289643638
C	0.51234803835535	1.11865182679963	-0.78311787196002
C	-0.04416904858590	-0.04213808846545	-0.09916447754514
C	-0.25965912094822	0.25725472196192	1.37182116958892
O	-0.34498562862655	1.36023476467747	1.87460680953996
O	-0.31161528317294	-0.89077318258695	2.06864007476107
H	-2.47425867284355	-1.46678623669041	3.55321384639594
H	-1.93894397567151	-0.65204109954929	5.03255457269287
H	-2.29534819210914	0.30042505457850	3.58420530549561
H	0.17472769628473	0.06839451037046	3.84661718952909
H	0.01934827365830	-1.70682752332638	3.88075213928843

H	1.59610517272435	0.85881784723288	-0.78065904939392
H	0.25439430022458	1.15144715355833	-1.84498629217873
H	0.42354032125526	2.09265344767041	-0.28537038382273

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Free carbene/B3LYP/6-311G(d)/RKS/30 degrees Constrained Optimization

C	-0.42896241466189	-0.68267491869687	3.56130640725129
C	-1.92154302142584	-0.66534304090949	3.84748130851590
C	0.89942350088701	0.92753657766713	-0.70703690523254
C	0.22569212655257	-0.15924512303396	-0.01783501045832
C	-0.19211863851038	0.20004715907590	1.35915581393706
O	-0.49645327068507	1.31696091935166	1.73436629944623
O	-0.15829003049416	-0.88849462572603	2.15116295680090
H	-2.39722186034232	-1.57661178151090	3.47675782428959
H	-2.09079188711797	-0.60626397962496	4.92705032907720
H	-2.39671995567568	0.19733290976409	3.37926397903203
H	0.04877514712537	0.24580565048133	3.88199353856218
H	0.06172666899376	-1.52701244489258	4.04600877190066
H	1.39057456189679	0.65461138066012	-1.64136431743537
H	-0.05532735761429	1.42940160563295	-0.99593512701553
H	1.45938872007210	1.67896031076161	-0.13266289767130

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Free carbene/B3LYP/6-311G(d)/RKS/40 degrees Constrained Optimization

C	-0.42517862453145	-0.74388817766892	3.53859928329568
C	-1.89650796265970	-0.64680038335238	3.90479291794113
C	0.94248357276039	0.88101808179041	-0.71886986177601
C	0.05564490172447	-0.07608050565874	-0.05538511312600
C	-0.19856719699443	0.18876134788344	1.36017127105226
O	-0.36930623931491	1.32403664136160	1.77500102658769
O	-0.25196076052788	-0.92482046114818	2.10936878508650
H	-2.44576889688746	-1.51737957106528	3.53844453903147
H	-2.00728734165757	-0.60470607059093	4.99277784865454
H	-2.34174645994211	0.25477813119198	3.48105985581881
H	0.12038042580495	0.14852119634509	3.85196127934927
H	0.04276808612855	-1.62630340145390	3.97599841824700
H	1.77475198572472	0.28996308530237	-1.14083091739438
H	0.44166397156329	1.25181698489453	-1.62316524216563
H	1.34098722080915	1.70930211116893	-0.12021111960233

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Free carbene/B3LYP/6-311G(d)/RKS/50 degrees Constrained Optimization

C	-0.41700814046288	-0.77291560269225	3.52416012894675
C	-1.88200999361891	-0.62640614020905	3.89760492383200
C	1.03383013782065	0.74677057383361	-0.72441166238029
C	-0.00286947844239	-0.04715942381155	-0.06979495439565
C	-0.17492697677690	0.16766424728861	1.35220732116753
O	-0.29025006371991	1.31022995295341	1.77261955185437
O	-0.25517134313259	-0.94888672281375	2.09175243239788
H	-2.46359705638214	-1.47423869502027	3.52778773588280
H	-1.98696559945823	-0.58776463037169	4.98631726149674
H	-2.29692089920137	0.29324657758585	3.48194349538387
H	0.16257705521285	0.09560882358389	3.84278890770771
H	0.02140106497872	-1.67502896494833	3.95175907409618
H	1.85448479502413	0.01860575411949	-0.89128066300094
H	0.74490860374865	1.05654245124231	-1.73297248508237
H	1.44582783341032	1.57997544125972	-0.14076809690658

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Free carbene/B3LYP/6-311G(d)/RKS/60 degrees Constrained Optimization

C	-0.41519434247371	-0.77775732144094	3.54081825209658
C	-1.88727997554166	-0.61969033601673	3.87853934645030
C	1.13339992866876	0.57740407944307	-0.72515775501309
C	-0.01115631969153	-0.04035482513421	-0.05796664067070
C	-0.12508403628144	0.12930511222014	1.36220341422450
O	-0.21243161947030	1.28532799120206	1.76008485511142
O	-0.22146531803306	-0.97409170827324	2.11339405142743
H	-2.46477531481460	-1.46931660061676	3.50645768439969

H	-2.01707991635234	-0.56621392536054	4.96394106437874
H	-2.28859716392153	0.29635724478387	3.44179252583019
H	0.16253632502335	0.09109275929888	3.86077539502416
H	0.00953158042803	-1.67618172343567	3.98923237585460
H	1.81974566960844	-0.27569374365626	-0.90362077570177
H	0.89134349122371	0.95081810790351	-1.72377522546450
H	1.68591711262787	1.32153546708283	-0.13700559694755

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Free carbene/B3LYP/6-311G(d)/RKS/70 degrees Constrained Optimization

C	-0.41371888528386	-0.78432745039348	3.54529896707643
C	-1.88800170304020	-0.61649485435892	3.86691974634253
C	1.20532229400750	0.38965394545324	-0.72221196372802
C	-0.02947073041425	-0.02370833355406	-0.05515842369872
C	-0.09869114910841	0.10874389453994	1.36491380367718
O	-0.15185067725886	1.27098741053530	1.75427024920944
O	-0.20712860253128	-0.98874890482216	2.11909964091960
H	-2.46665556872746	-1.46458307342508	3.49328082823559
H	-2.02849903211927	-0.55661142942626	4.95061234170179
H	-2.28025185343730	0.29954705253151	3.42179727494872
H	0.16689210520246	0.08178825646505	3.86614519491257
H	0.00181183019158	-1.68323714386757	4.00100613679632
H	1.73824423569454	-0.57213471362807	-0.87024383163654
H	1.04391132940715	0.78521561797051	-1.72791874851788
H	1.87154291141767	1.03787041298005	-0.13809824523902

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Free carbene/B3LYP/6-311G(d)/RKS/80 degrees Constrained Optimization

C	-0.41241649273735	-0.79288931390954	3.54053348275318
C	-1.88660002188874	-0.61698551690072	3.85751837680905
C	1.24691447808482	0.18635586927070	-0.71621274631404
C	-0.04720633809995	0.00230706934906	-0.05586813711616
C	-0.08607578359694	0.10992967426744	1.36503050772872
O	-0.10640891298723	1.27099043144146	1.76036214812319
O	-0.20239428849748	-0.99104267804204	2.11259751997688
H	-2.46965872816718	-1.45940851600624	3.47797763833680
H	-2.03050050863128	-0.56117384516304	4.94095007884625
H	-2.27180231271584	0.30365671015516	3.41557029881164
H	0.17374220050467	0.06682960226297	3.86737499569114
H	-0.00432984806234	-1.69720847286264	3.99211608650360
H	1.61094529337634	-0.85823228531938	-0.80412934805838
H	1.17232490965628	0.56095254767369	-1.73944133498231
H	2.00663875476221	0.73585250378311	-0.14466659610958

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Free carbene/B3LYP/6-311G(d)/RKS/90 degrees Constrained Optimization

C	-0.41108277843724	-0.79817700899412	3.53141725626938
C	-1.88592216446185	-0.62394746593276	3.84599034204618
C	1.25617423060536	-0.02762904851207	-0.70667737318817
C	-0.05446404321924	0.03276431096423	-0.05604932949752
C	-0.07540669349880	0.13464874684795	1.36714346848601
O	-0.07077109151675	1.28832463199789	1.77932140798144
O	-0.19737257401765	-0.97691399695947	2.10095627332192
H	-2.46939739105865	-1.46047749081120	3.45418858967406
H	-2.03334873579839	-0.58117938633588	4.92953582411879
H	-2.26876963764691	0.30277263143139	3.41457649116789
H	0.17614918072033	0.05559721832108	3.87093747926606
H	-0.00587598547878	-1.70942972741210	3.97155026219129
H	1.42132738899419	-1.12545176590186	-0.73241475124160
H	1.25713915074893	0.30137146761694	-1.74784483096484
H	2.10319913506545	0.39930127967998	-0.15291813863091

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Free carbene/B3LYP/6-311G(d)/RKS/100 degrees Constrained Optimization

C	-0.40790113615002	-0.80155152981138	3.52043052602986
C	-1.88548593552319	-0.63424586376710	3.82611655680065
C	1.22706976667439	-0.24506232204792	-0.69288443754699
C	-0.05320097845893	0.05958041457021	-0.05360751556614

C	-0.05753966910951	0.17543864881223	1.37363931662951
O	-0.03704665111038	1.31629478846644	1.81173373244503
O	-0.18205092771273	-0.95287453580612	2.08880967335591
H	-2.46523068069356	-1.46400555628248	3.41477925575739
H	-2.04192034558351	-0.61073565220674	4.90897755071478
H	-2.26611537394863	0.29971488872604	3.40838920861258
H	0.17605957968407	0.04596260390491	3.88004637499436
H	-0.00561876281994	-1.72063013637268	3.94691703097041
H	1.18041252340804	-1.35508777126672	-0.65024715776032
H	1.28154658436784	0.01480024771335	-1.75183454001719
H	2.14422450197605	0.04313817936795	-0.16155260441983

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Free carbene/B3LYP/6-311G(d)/RKS/110 degrees Constrained Optimization

C	-0.40385530441695	-0.80307176577676	3.51155987385726
C	-1.88716230289800	-0.64686254442865	3.79546406547073
C	1.15636150765990	-0.45821432926295	-0.67720165440726
C	-0.04584482209308	0.07924827369771	-0.04530362634833
C	-0.02349820324935	0.22048417221087	1.38627174801650
O	0.00984546728664	1.34567630947631	1.85395098960051
O	-0.15314075323503	-0.92640736050303	2.08211777864810
H	-2.45684885581108	-1.47156361204496	3.36046913336725
H	-2.06191536153939	-0.64218764395393	4.87574747103569
H	-2.26506669384383	0.29264132195279	3.38757273380066
H	0.17067731789882	0.03982060836135	3.89585741345996
H	-0.00526008468565	-1.72835013133507	3.92825960096544
H	0.90594853146775	-1.53646301000458	-0.55862587615708
H	1.23138862793104	-0.28115619873024	-1.75167148575476
H	2.12249977352821	-0.31454894865887	-0.17475519455466

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Free carbene/B3LYP/6-311G(d)/RKS/120 degrees Constrained Optimization

C	-0.40051651121722	-0.80342268211792	3.50718810628544
C	-1.89109952404116	-0.65837954169809	3.75833485381531
C	1.04800748310442	-0.65794427909635	-0.66128598977603
C	-0.03759717077514	0.08599883093426	-0.03321794505981
C	0.02180567343715	0.25435680946038	1.40148109590230
O	0.06304659132913	1.36513594556207	1.89478832800043
O	-0.11589389326552	-0.90773323750794	2.08361571286447
H	-2.44618675294603	-1.48159331051675	3.30204033674772
H	-2.09106435129457	-0.66537587143301	4.83418700355437
H	-2.26522517097079	0.28315957156348	3.35140662706976
H	0.16025727205569	0.03793550055345	3.91409232672473
H	-0.00685066110796	-1.73146605001012	3.92274415993337
H	0.61980401123516	-1.66849678265844	-0.46888254591262
H	1.11293236667735	-0.55758004642402	-1.74607179093117
H	2.04045026077948	-0.65765837161099	-0.19070730821829

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Free carbene/B3LYP/6-311G(d)/RKS/130 degrees Constrained Optimization

C	-0.39968530307339	-0.80512165433426	3.50262443307108
C	-1.89518460861598	-0.66479531262884	3.72741889822881
C	0.91481739491566	-0.83657201627311	-0.64416802417174
C	-0.03393274906756	0.08118915747776	-0.02868252325630
C	0.05803729548358	0.27102185009619	1.40932476140741
O	0.09694111749557	1.37110350541489	1.92126904901091
O	-0.08852311614990	-0.90059449575091	2.08500600398588
H	-2.44013880834848	-1.48791552226896	3.25874078410251
H	-2.11459051434985	-0.67575939793801	4.79941452453397
H	-2.26474891758310	0.27714816055876	3.31713875982947
H	0.15149129878324	0.03536114999065	3.92396610732801
H	-0.01193232800059	-1.73463807445582	3.92078720228963
H	0.33297219973518	-1.75479700293007	-0.39706260803944
H	0.96384491498900	-0.79315845976506	-1.73342731141941
H	1.90571015678662	-0.97973979519319	-0.19263708590079

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Free carbene/B3LYP/6-311G(d)/RKS/140 degrees Constrained Optimization

C	-0.40137051471302	-0.81184081225772	3.49535444894964
C	-1.89754235465521	-0.66217918560375	3.71160961919246
C	0.76794232067450	-0.98878952188940	-0.62750504529434
C	-0.03776544797695	0.07054503770427	-0.03902572042371
C	0.06916700501843	0.27176568721990	1.40595819967658
O	0.09151962636765	1.36492699635767	1.93019996198248
O	-0.08080428680615	-0.90455992392751	2.08045769960754
H	-2.44521279905038	-1.48116831275647	3.23875129793541
H	-2.12313366905196	-0.67371705943023	4.78225882259945
H	-2.25877002254182	0.28283072152584	3.30116041864138
H	0.15228935326113	0.02361246033596	3.92327506763842
H	-0.02313353571791	-1.74552849692757	3.91311813474592
H	0.04766038026609	-1.79676624528744	-0.35924403699592
H	0.81842998172661	-0.98191503660932	-1.71749282057541
H	1.72382662919900	-1.27543747345421	-0.16916307667991

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Free carbene/B3LYP/6-311G(d)/RKS/150 degrees Constrained Optimization

C	-0.40561611483886	-0.82156988175171	3.48554790632899
C	-1.89862186634937	-0.65354498152241	3.71211192512059
C	0.60929161375956	-1.11412709375268	-0.61231296617541
C	-0.04322702960484	0.06484839069936	-0.06400912971623
C	0.05685367026867	0.26543148407777	1.39438580027023
O	0.05726501079753	1.35392314875873	1.92642606909571
O	-0.09345372296340	-0.91196489954912	2.06919419534726
H	-2.45969203813626	-1.46452621573639	3.24098302015350
H	-2.11705225509263	-0.66585755989839	4.78420527694256
H	-2.25078819435258	0.29720302448793	3.30735136863632
H	0.16069826141908	0.00510833292829	3.91416989242257
H	-0.03765243235948	-1.76210445890048	3.89722618616074
H	-0.24146084733858	-1.79245503200679	-0.36659979985156
H	0.69255720004327	-1.12968215156292	-1.70038900207814
H	1.49029834674789	-1.54500343327121	-0.11857777165711

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Free carbene/B3LYP/6-311G(d)/RKS/160 degrees Constrained Optimization

C	-0.41225156457437	-0.83275244500927	3.47531227585448
C	-1.89837439793254	-0.64069907678433	3.72829284618694
C	0.44100185263230	-1.20972998819743	-0.60248591170354
C	-0.03877695239510	0.06855219140935	-0.101111012897412
C	0.02356314797006	0.25432996273976	1.37780393712562
O	0.00202749462306	1.34004808207174	1.91316065069192
O	-0.12367596573883	-0.92053648053968	2.05434721276907
H	-2.48078954439469	-1.44006477370536	3.26312921093860
H	-2.09811201629133	-0.65591757107877	4.80395605075063
H	-2.24161955115077	0.31806815159724	3.33535424702189
H	0.17430984577225	-0.01754122952072	3.89920678339452
H	-0.05431280695270	-1.78164406557267	3.87654878369660
H	-0.53006348955760	-1.72966522356040	-0.42034994299428
H	0.59017443861863	-1.24880423834070	-1.68312558896700
H	1.19771922037164	-1.78201102550875	-0.05032745479135

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Free carbene/B3LYP/6-311G(d)/RKS/170 degrees Constrained Optimization

C	-0.42133040308387	-0.83952436884293	3.46908935866219
C	-1.89805300426625	-0.62961571155149	3.76054902939553
C	0.26323141832120	-1.27429760661733	-0.60301384977001
C	-0.00729128327273	0.07904668696889	-0.14318193701210
C	-0.02657910643547	0.23991930288936	1.36021770705078
O	-0.06083929681180	1.32571431217295	1.89219634647370
O	-0.16935896412968	-0.92811992195824	2.04157343463311
H	-2.50172290584184	-1.42096039091511	3.30891928090275
H	-2.06972227554503	-0.64592658335224	4.84100448111069
H	-2.23947417020983	0.33446785832931	3.37952433618882
H	0.18507251440385	-0.03120246091449	3.87884992124989
H	-0.06542356461862	-1.79312802141162	3.86080858309883
H	-0.80499100047614	-1.59724095464834	-0.53348369231793
H	0.51311535052274	-1.34967100601358	-1.66316247808635

H 0.83015949544347 -1.97754476013513 0.01982244842010

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Free carbene/B3LYP/6-311G(d)/RKS/180 degrees Constrained Optimization

C -0.43097209108481 -0.83914878623441 3.47110679191680
C -1.89590112885318 -0.62050769184852 3.81118071562387
C 0.07288790325485 -1.30616064727745 -0.62098141340515
C 0.05174661292110 0.07743785173138 -0.16819998916712
C -0.09758808690636 0.22358949624286 1.34537193853445
O -0.13109576194518 1.31214279524648 1.86974160197635
O -0.22785122429601 -0.93602299986448 2.03671318261192
H -2.51805985681101 -1.41063570485420 3.38318106979697
H -2.03081208474614 -0.63222990293108 4.89686069205372
H -2.24443759543713 0.34407821754312 3.43820412235987
H 0.19165859483609 -0.02981232080804 3.85473016631972
H -0.06602784921889 -1.79171638424532 3.85689382358049
H -1.03574607220790 -1.40246327602399 -0.73574668819934
H 0.46655710828095 -1.43586961388358 -1.63153872458739
H 0.37407495221363 -2.10917024979277 0.06219568058483

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Free carbene/B3LYP/6-311G(d)/RKS/190 degrees Constrained Optimization

C -0.41090457077101 -0.81389359013374 3.48057632387568
C -1.87531012108512 -0.65295059964343 3.85334291342944
C 0.04102245497842 -1.31297153833606 -0.63442674043535
C 0.21581625875284 0.04407588713866 -0.13191356313199
C -0.15433037142041 0.22170893333723 1.33262790211592
O -0.23274466196885 1.31588657066434 1.84222480724849
O -0.24001055139460 -0.93199594090876 2.04468276238444
H -2.47182511155590 -1.47894287186169 3.45777471786633
H -1.98287895059535 -0.64657900939951 4.94214984086058
H -2.27374501294436 0.28711831586720 3.46816755864762
H 0.18175819848774 0.03325427183266 3.82996704547016
H 0.00744611901593 -1.73949727975307 3.87777129932260
H -0.98372111630552 -1.20397748295843 -1.06468873851314
H 0.66785209149449 -1.53078930622196 -1.50314558080343
H -0.00999123468830 -2.14693557662346 0.07460242166264

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Free carbene/B3LYP/6-311G(d)/RKS/200 degrees Constrained Optimization

C -0.39454140402837 -0.79281633973739 3.48183643221868
C -1.85052375159991 -0.68493028279679 3.90379217115906
C 0.00737402317520 -1.30647537854117 -0.66016316507506
C 0.33058192941828 -0.01879577616168 -0.05164326339935
C -0.21899228989328 0.22266767948983 1.31669734589111
O -0.34826432476300 1.31989021911464 1.81293937861210
O -0.27194050959198 -0.93119005175243 2.04389462662284
H -2.42573079061230 -1.54196792374606 3.54427914161375
H -1.92067280614481 -0.66150827386691 4.99554332955878
H -2.29877675538322 0.23050376857299 3.51444530565479
H 0.17178653428645 0.08672515087221 3.79418943633736
H 0.07729734159472 -1.69143129744029 3.88141107603886
H -0.79857321885878 -1.02699038073157 -1.37460381879206
H 0.81138054527877 -1.65946388377596 -1.31318035942228
H -0.39197110287775 -2.10070644649943 -0.01972466701858

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Free carbene/B3LYP/6-311G(d)/RKS/210 degrees Constrained Optimization

C -0.38571872521994 -0.77367291662617 3.49129087462080
C -1.84106929094951 -0.71564194478509 3.92448385184450
C -0.00496168379921 -1.29294530857471 -0.68233179089393
C 0.42110903884207 -0.08466276837808 0.01985690169747
C -0.22703499681624 0.21314285338738 1.30989434314009
O -0.41414841489093 1.31572976738222 1.77497922687439
O -0.27421200269448 -0.93528864800583 2.05440208586881
H -2.38503080535160 -1.60116168101145 3.58596526799310
H -1.90317064654655 -0.67442142294055 5.01632079342288
H -2.32745454964555 0.17386300091796 3.52111447461914

H	0.14661159795894	0.13460286567913	3.78031958013108
H	0.12627669121365	-1.64407040343458	3.90388119473105
H	-0.69265921152309	-0.89241079580476	-1.45844137439372
H	0.80903029265461	-1.73981032930010	-1.26036048462886
H	-0.56913387323215	-2.03974148550537	-0.11166197502682

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Free carbene/B3LYP/6-311G(d)/RKS/220 degrees Constrained Optimization

C	-0.37908596851626	-0.75351530344270	3.51527435621608
C	-1.84171824100842	-0.74347185130701	3.92613500118929
C	-0.01307375988040	-1.27526874154267	-0.70513979451072
C	0.49772296738288	-0.14533409034481	0.06826512111009
C	-0.19471099940016	0.18432414508417	1.31391450178634
O	-0.43891815996918	1.29585065548454	1.72882502872850
O	-0.24225264911493	-0.94689513840977	2.08356114084034
H	-2.34501978787496	-1.65781074392756	3.60162085465164
H	-1.92242976946079	-0.67856820142693	5.01565878267341
H	-2.35658402561059	0.11580243849566	3.49346710866698
H	0.11239006879389	0.18234246721161	3.78764768709411
H	0.16148553138702	-1.59168005832406	3.95714283871681
H	-0.68862051673507	-0.78264553472510	-1.43741779535125
H	0.75632218588981	-1.75417302706722	-1.31585134379275
H	-0.62707345588284	-2.00544623275816	-0.16339051801888

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Free carbene/B3LYP/6-311G(d)/RKS/230 degrees Constrained Optimization

C	-0.37038581727181	-0.73162255079650	3.55017804259216
C	-1.84348890693693	-0.77123074300447	3.91836889622107
C	-0.02996538532747	-1.25039864499780	-0.73170953051662
C	0.55806729170388	-0.19984236706989	0.09823249534054
C	-0.14432625503093	0.13881560499400	1.32729502250717
O	-0.44524495340100	1.25866781082662	1.68094633085287
O	-0.18303516558521	-0.96461898043950	2.12885832884209
H	-2.29824606190393	-1.71594724881038	3.60955889762397
H	-1.95973629554484	-0.67590252952620	5.00245758587570
H	-2.38085448515367	0.05119594903090	3.44333456874862
H	0.07409317431904	0.23196425633740	3.80540128225891
H	0.19145226512762	-1.53157033121219	4.03413652470861
H	-0.72613914113668	-0.68440497930200	-1.38679078149978
H	0.68597437957938	-1.72423188172673	-1.40675630235806
H	-0.64973122343746	-1.98736258130326	-0.20379839119725

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Free carbene/B3LYP/6-311G(d)/RKS/240 degrees Constrained Optimization

C	-0.35937109843067	-0.70625650839533	3.59171735324385
C	-1.84201228891860	-0.80225077287454	3.90589411509418
C	-0.05723240600659	-1.21810007581285	-0.76099397285679
C	0.60531830693444	-0.25364826828660	0.11807248887723
C	-0.08689283871373	0.08132933272294	1.34677017815199
O	-0.44280991885096	1.20646379101025	1.63259056340779
O	-0.10462028543421	-0.98473979172813	2.18777249293396
H	-2.24008029016385	-1.77861047684654	3.61789578681258
H	-2.00486664767302	-0.67205014541401	4.98032333948707
H	-2.39856100799362	-0.02500423245975	3.37946910602147
H	0.03110428246518	0.28564926593792	3.82501404689780
H	0.21964475307474	-1.45984733585650	4.12681476553680
H	-0.77689269371651	-0.58968816081803	-1.32608517485199
H	0.60465732325339	-1.66473217389119	-1.50548877614932
H	-0.66895176982599	-1.97500366428766	-0.25005334260664

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Free carbene/B3LYP/6-311G(d)/RKS/250 degrees Constrained Optimization

C	-0.35495975990893	-0.67436434210893	3.63705951221896
C	-1.84637544265251	-0.81251534052967	3.88612780949434
C	-0.08731655822517	-1.19579501317456	-0.78791067657300
C	0.65681671241207	-0.33817360224604	0.13815331524172
C	-0.01386038926244	0.00106005719565	1.36978189556034
O	-0.40440060678299	1.13513764158216	1.57660702077188

O	-0.02068154120585	-1.01314257502372	2.26208270883613
H	-2.19415795347008	-1.81630199835175	3.62898534310062
H	-2.06614360337985	-0.63698344190436	4.94381342891792
H	-2.40548365041283	-0.08382739761909	3.29645856814385
H	-0.01111349445572	0.34141466643790	3.83755271325678
H	0.22451022879444	-1.37777338503928	4.23586971272857
H	-0.81975953182033	-0.50545222906696	-1.25279845895825
H	0.51630983880786	-1.60572768666911	-1.59945274328374
H	-0.69495082843767	-1.97404457048226	-0.30261717945614

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Free carbene/B3LYP/6-311G(d)/RKS/260 degrees Constrained Optimization

C	-0.35270882584182	-0.64142432851459	3.67925086230318
C	-1.84725009826312	-0.81906369792836	3.87852576837149
C	-0.11392150637017	-1.16843904398791	-0.82117769335719
C	0.69656364441971	-0.43873548832214	0.16021261886654
C	0.04331883708089	-0.09285400384776	1.39144472326234
O	-0.37333366165924	1.04767837853614	1.51607762979617
O	0.04964735120239	-1.04561569465737	2.33964430506566
H	-2.15039193075910	-1.84710775922744	3.66438997052623
H	-2.11548216168746	-0.59437424087925	4.91546051333679
H	-2.40730073409393	-0.14406801953261	3.22868405810107
H	-0.04994040043719	0.39480282035528	3.83502153375597
H	0.22545536078308	-1.28966124701796	4.33828033193443
H	-0.84354843382587	-0.41983163223037	-1.18515466833898
H	0.44463522497690	-1.52641289749706	-1.68722998509092
H	-0.72730924552505	-1.97138236224862	-0.38371699853280

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Free carbene/B3LYP/6-311G(d)/RKS/270 degrees Constrained Optimization

C	-0.34976041226593	-0.60624355204111	3.71370332153371
C	-1.84056471283085	-0.83371673248802	3.88871371103300
C	-0.13557702209096	-1.14588533627680	-0.85383239621136
C	0.71465937759736	-0.54921047828797	0.18264042077079
C	0.07126944050836	-0.17983108075316	1.40721045676774
O	-0.37356025153569	0.95850929506473	1.45776225350031
O	0.10264927208292	-1.06923181409965	2.40919904222591
H	-2.09703145858634	-1.88343975381706	3.72427232590969
H	-2.14340209262091	-0.56429383895389	4.90519813471108
H	-2.41148311888067	-0.21877271838428	3.19034510715834
H	-0.09072283945590	0.44792420454801	3.81777658026001
H	0.23661955065245	-1.19315045681930	4.42102902665622
H	-0.78164617121027	-0.30728119875266	-1.17472901449551
H	0.40751802082367	-1.49480402012131	-1.73317771008047
H	-0.83053416218725	-1.91706173581754	-0.48685328973948

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Free carbene/B3LYP/6-311G(d)/RKS/280 degrees Constrained Optimization

C	-0.34459781899595	-0.57306975710175	3.73973482428777
C	-1.82637279403193	-0.85775117315696	3.90876158658293
C	-0.15362250415918	-1.13039734064585	-0.88228871604584
C	0.70799361815156	-0.65335767788295	0.20272727185775
C	0.06861390607567	-0.24460880533893	1.41696710065053
O	-0.41962041460399	0.87788436918535	1.41262360398921
O	0.14700227411485	-1.07519118225720	2.46439988351707
H	-2.03464296270346	-1.92410706388874	3.79019243922438
H	-2.15287333296850	-0.55645943321270	4.90881968698366
H	-2.41518696075881	-0.30074266428641	3.17740334395644
H	-0.13206869331016	0.49475270921883	3.79849245251969
H	0.25692421535250	-1.10132918409313	4.47972635054103
H	-0.62903259553143	-0.18903532003522	-1.21779578403209
H	0.38973111367292	-1.53184003259446	-1.73899121296024
H	-0.98381363030410	-1.79123666090989	-0.59105986107233

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Free carbene/B3LYP/6-311G(d)/RKS/290 degrees Constrained Optimization

C	-0.34197089294676	-0.54191598265422	3.75594620527779
C	-1.81081044703992	-0.88756957805532	3.92664642736942

C	-0.16995702634069	-1.11423873942146	-0.90419084533921
C	0.69281815398145	-0.75847016050197	0.22155633079742
C	0.05998852827715	-0.28959911837019	1.42123168195055
O	-0.46369146610815	0.81553093314758	1.37868210620845
O	0.18262345265259	-1.06851944318159	2.50492634850461
H	-1.96927077054886	-1.96603851682881	3.84699455697135
H	-2.15953730764661	-0.56419407637376	4.91218308574228
H	-2.41936072450793	-0.38629362768316	3.17136201760550
H	-0.17833510864053	0.53573494167682	3.77651273810861
H	0.27642312270552	-1.01404497890159	4.51958125292378
H	-0.46166097664117	-0.10137828716885	-1.24430075295730
H	0.35372666518696	-1.58124597278092	-1.73961894965540
H	-1.11255178238303	-1.63424660990260	-0.67779923350788

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Free carbene/B3LYP/6-311G(d)/RKS/300 degrees Constrained Optimization

C	-0.34163737148419	-0.51079502391298	3.76569714273253
C	-1.79326780016652	-0.92337297725687	3.93732008685703
C	-0.18837511454444	-1.09863805378085	-0.91600469058761
C	0.67078420218901	-0.85590228007319	0.23827421161878
C	0.04935887908012	-0.31590515270236	1.42216414485046
O	-0.51186042421159	0.76783171964184	1.35225423596802
O	0.21991836231828	-1.04559685959670	2.53568186192458
H	-1.89769303085946	-2.01020403375109	3.88807425427761
H	-2.16415126283125	-0.58938594191413	4.91109177674721
H	-2.42080637519979	-0.47468284007856	3.16466285606496
H	-0.23058763652079	0.57358655398731	3.75681785385683
H	0.29249884577499	-0.93051870074651	4.54684354568512
H	-0.28641335325585	-0.04944961580834	-1.26132050830997
H	0.29499238650421	-1.63957257972981	-1.73091906316698
H	-1.21432688679273	-1.45388343127777	-0.74092473851858

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Free carbene/B3LYP/6-311G(d)/RKS/310 degrees Constrained Optimization

C	-0.34649579585947	-0.47836984640615	3.76850938425377
C	-1.7785369988019	-0.95702834887545	3.93652769769933
C	-0.20846203995455	-1.09035792775090	-0.91299704646861
C	0.64736892019177	-0.96428703277079	0.25881357912588
C	0.04720896020670	-0.32811770731285	1.41991071689239
O	-0.53633827071286	0.73957382172481	1.32936196765770
O	0.25262996407205	-1.01443707047686	2.55837810915496
H	-1.82956236789143	-2.04851893312064	3.91374971693590
H	-2.17610116853253	-0.61745421727639	4.89770008245730
H	-2.41951317302487	-0.55897191397707	3.14716120960608
H	-0.28788552948455	0.60949689135778	3.73382043484772
H	0.29826143792329	-0.84800260452972	4.56610036149899
H	-0.09626305962063	-0.04126998467404	-1.26190610883894
H	0.20019417107736	-1.71265119474139	-1.71042201246991
H	-1.28807162851006	-1.24609314817034	-0.77499512235258

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Free carbene/B3LYP/6-311G(d)/RKS/320 degrees Constrained Optimization

C	-0.35179669116272	-0.45017522834458	3.76872610407026
C	-1.76374974980815	-0.98340076472319	3.94540910211403
C	-0.21765012063035	-1.07817505449895	-0.91676835209086
C	0.61518014618283	-1.06198819222685	0.27564590137129
C	0.02822242429886	-0.34450862687308	1.41418508957638
O	-0.58985890572487	0.69967552778299	1.30800384376812
O	0.27150582921069	-0.98752622975730	2.57248483015557
H	-1.76967248656317	-2.07625500840629	3.94814101827019
H	-2.17711819841725	-0.63799233252764	4.89771713230001
H	-2.41908217099203	-0.63056878476081	3.14637355900208
H	-0.33788063703542	0.63814219905377	3.70955806597913
H	0.30517612952751	-0.77570443434921	4.57550223550738
H	0.08034217091009	-0.05969342239427	-1.25522479950797
H	0.11682730153506	-1.75723362601354	-1.70216985378315
H	-1.31201162133108	-1.05108523896107	-0.81787090673247

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Free carbene/B3LYP/6-311G(d)/RKS/330 degrees Constrained Optimization

C	-0.35720403042508	-0.42651703334153	3.76801589657587
C	-1.7496869354137	-0.99980496064763	3.97403464887939
C	-0.20948040344116	-1.05787408053600	-0.93688594497443
C	0.57539860842053	-1.14972292769206	0.28292697635520
C	-0.01749239082056	-0.37745769900917	1.40558371478843
O	-0.68407401633020	0.63309412998506	1.28709167097394
O	0.27017827384263	-0.97311569291675	2.57885159748501
H	-1.72009351673677	-2.09179776525412	4.00467762072458
H	-2.16323953772128	-0.64317001096479	4.92204140245734
H	-2.42469436309127	-0.68865373554854	3.17420801910582
H	-0.37952937060014	0.6599595779636	3.68163455758718
H	0.31806918635242	-0.71120958509202	4.57509298352722
H	0.24574731902116	-0.08662227455504	-1.24617532532721
H	0.06626485823400	-1.76751014929091	-1.71804866861211
H	-1.29173020316290	-0.87612338993288	-0.88333617954623

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Free carbene/B3LYP/6-311G(d)/RKS/340 degrees Constrained Optimization

C	-0.36430983256717	-0.40679532708803	3.76451819959037
C	-1.73615577157057	-1.00845460158007	4.02319296855657
C	-0.18322914174224	-1.02578112922630	-0.97251677535429
C	0.52691166118252	-1.23397262273323	0.27772423091824
C	-0.09018618539651	-0.43219826984562	1.39449204697715
O	-0.81025892813962	0.53805364984006	1.26680819210906
O	0.24800763871254	-0.97464657243623	2.57807083261581
H	-1.67669612403074	-2.09769794584487	4.08759253738295
H	-2.13497359591348	-0.63198847418109	4.96978616820801
H	-2.43832990078304	-0.74038144915245	3.23143079006276
H	-0.41830934090306	0.67569213274441	3.64476113274972
H	0.33721910991766	-0.64872253784399	4.56306425520229
H	0.40580961609871	-0.11200762783160	-1.23474773684480
H	0.04842821462036	-1.74577751041406	-1.75879319824161
H	-1.23549399948534	-0.71181093140692	-0.96567067393222

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Free carbene/B3LYP/6-311G(d)/RKS/350 degrees Constrained Optimization

C	-0.37319337617321	-0.39166674373122	3.75536452567922
C	-1.72236996518404	-1.01094544356068	4.08335074247829
C	-0.14069950480104	-0.98142699551937	-1.01293585211052
C	0.46935935369937	-1.31497071228202	0.26302389456020
C	-0.18364976167161	-0.50670074088313	1.38154908912771
O	-0.95760650222870	0.41910848723286	1.24862796011334
O	0.21113595269117	-0.99057248295010	2.57036740104974
H	-1.63704356820747	-2.09548756516571	4.18572679947882
H	-2.09591745253384	-0.60720660813566	5.02901620737956
H	-2.45640510625526	-0.78661889036675	3.30731906781654
H	-0.45617608884145	0.68449088520300	3.59769172168090
H	0.35985023233830	-0.58911935030565	4.53763563127090
H	0.55838540007759	-0.13273501070598	-1.22151522553662
H	0.05360884501787	-1.69965365091416	-1.81147385173311
H	-1.15084503792768	-0.55298439491543	-1.04403514125498

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Free carbene/B3LYP/6-311G(d)/RKS

/0 degrees Constrained Optimization

C	0.00784257708064	-1.36781665546565	3.38623110847995
C	-1.40732823584203	-1.29984826143851	3.93778391704083
C	-0.00213751053426	0.98188362788344	-1.03633151548230
C	0.01256819350187	-0.08416779120675	-0.03839035027071
C	-0.01449857682210	-0.06883316545884	1.38913777595780
O	-0.05901378636948	0.97419294863113	2.03030901043374
O	0.02011161746687	-1.30341051409349	1.94039682468136
H	-2.03320759350360	-2.07996495420536	3.49713360646808
H	-1.39368878393813	-1.44485059876810	5.02245021975049
H	-1.85893430579400	-0.32800696766670	3.73105444932538
H	0.62608735117619	-0.56064466800707	3.78278667579372

H	0.47970049207664	-2.32488933013934	3.61180768922724
H	-0.88721441491519	0.91766952429478	-1.68325848618421
H	-0.00447944875946	1.96564859669368	-0.54758637038204
H	0.87188320017603	0.92809215494675	-1.69825442183932

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Free carbene/B3LYP/6-311G(d)/BSS/10 degrees Constrained Optimization

C	-0.00781837672941	-1.43586261424484	3.32033592257988
C	-1.35319259365582	-1.20033328551954	3.98778114273479
C	0.11567135133220	0.97108844418197	-0.99859717177681
C	-0.14143531493726	-0.18548820254101	-0.13400807883545
C	-0.03821028317116	-0.14162826193536	1.31958158482758
O	0.09657455559851	0.89414947123754	1.94962736525179
O	-0.11214819087619	-1.36642597610828	1.87729367422681
H	-2.10287135437343	-1.89789785281239	3.60620051926157
H	-1.26485198181623	-1.35090481482347	5.06806149388776
H	-1.70084530454022	-0.18042810185983	3.81461614863469
H	0.73415507813258	-0.70977670769190	3.65698310989852
H	0.36251883697207	-2.44386644796001	3.50991554588733
H	-0.22637909771278	0.81076400371095	-2.02384043494263
H	-0.36983034405700	1.86987423608222	-0.59216209670185
H	1.19286180883415	1.19991272328394	-1.03651859193396

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Free carbene/B3LYP/6-311G(d)/BSS/20 degrees Constrained Optimization

C	-0.00483823582050	-1.42700665276437	3.32225010175648
C	-1.35913694190635	-1.21948115761036	3.98064596212680
C	0.28808352285401	0.93263166433630	-0.99644275084712
C	-0.14016429550898	-0.16573927743323	-0.12538310592258
C	-0.04348888738939	-0.12674095738999	1.32572234681570
O	0.05975918346919	0.91006130599971	1.96088545554834
O	-0.10141510776999	-1.35550033517794	1.87863484752328
H	-2.09229606819788	-1.93074542378253	3.59235926768248
H	-1.27545787400225	-1.37039214869021	5.06130227031645
H	-1.72511059142520	-0.20622894888865	3.80648958792991
H	0.72015146322165	-0.68719580490228	3.66614418221621
H	0.38416110729040	-2.42799717539539	3.51174112865647
H	-0.19109018818107	0.90150487664519	-1.97827015804456
H	0.08959586287225	1.90159541417434	-0.51775530592426
H	1.37691597149411	0.89010426687936	-1.16305369683359

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Free carbene/B3LYP/6-311G(d)/BSS/30 degrees Constrained Optimization

C	-0.00348218465837	-1.42283693004726	3.32043594234760
C	-1.36069284101296	-1.22930777364197	3.97659054699637
C	0.44812677398740	0.86808554842633	-0.98790558519374
C	-0.15092244226712	-0.15322914459047	-0.12434798373281
C	-0.04848034269610	-0.12180584052120	1.32492361785061
O	0.03882610705261	0.91761807145494	1.95843931481464
O	-0.10012615139166	-1.35102231586727	1.87614237010919
H	-2.08626460115495	-1.94721671984567	3.58639056151514
H	-1.27744773835390	-1.38010581509300	5.05734992926677
H	-1.73586415775834	-0.21951600752803	3.80218819122798
H	0.71343622975180	-0.67572067549941	3.66561614137644
H	0.39576073870095	-2.41987539279845	3.50923270594055
H	-0.07809045572096	0.97486495944879	-1.94026811153958
H	0.49437442446382	1.83704341769008	-0.47247739167424
H	1.48859554705780	0.59166927541258	-1.22704011630494

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Free carbene/B3LYP/6-311G(d)/BSS/40 degrees Constrained Optimization

C	-0.00724076273233	-1.43144609499857	3.30921641174057
C	-1.35615288824851	-1.22863235674906	3.97886793965430
C	0.58850333994294	0.77674700357587	-0.98041443561476
C	-0.18187132666302	-0.13119466346790	-0.12572014240271
C	-0.05310691942859	-0.12099366808857	1.31980537484134
O	0.05239912324557	0.91712075851771	1.95287885294887
O	-0.11791689668709	-1.35093852721097	1.86542538917182

H	-2.09221877942140	-1.93741664874338	3.59171413471975
H	-1.26426844421183	-1.38591234828468	5.05803272230721
H	-1.72302458821130	-0.21438688068691	3.81293317536431
H	0.72012790980650	-0.69300357497973	3.65101914487107
H	0.38470647387927	-2.43312916459739	3.48835087977842
H	0.11076901780704	0.96154327325737	-1.94563660537896
H	0.77788104765833	1.72750850671929	-0.46302940370840
H	1.57900086726442	0.33727743873694	-1.18817330529285

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Free carbene/B3LYP/6-311G(d)/BSS/50 degrees Constrained Optimization

C	-0.01219336927874	-1.44172170656695	3.29821101014023
C	-1.35342049069377	-1.22744648282654	3.97888863879858
C	0.70975715616813	0.66213174182995	-0.97300214461044
C	-0.20998558231982	-0.10005632731220	-0.12281387061821
C	-0.05367913896851	-0.11847657578058	1.31705112367012
O	0.07379653950877	0.91699502353360	1.95047997324327
O	-0.13309611195221	-1.34984895369627	1.85475223653907
H	-2.10088061722695	-1.92443313346092	3.59219731623718
H	-1.25568213667939	-1.39337115116618	5.05625574298775
H	-1.70905949071538	-0.20770247792683	3.82246485981932
H	0.72686761284582	-0.71472597068022	3.63912392191083
H	0.36941122628006	-2.44917273042725	3.46683189862216
H	0.29268983656811	0.90385564579631	-1.95299253715110
H	1.03329176430309	1.57962364789803	-0.46092607771610
H	1.62670998616080	0.07116216178602	-1.14125195987268

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Free carbene/B3LYP/6-311G(d)/BSS/60 degrees Constrained Optimization

C	-0.01759318097361	-1.45061979320114	3.29170001825531
C	-1.35604519137685	-1.22917957267604	3.97496648793110
C	0.80754027706558	0.53195738029872	-0.96578338930744
C	-0.22965279765737	-0.05613554875526	-0.11191426613856
C	-0.04475366952936	-0.11366860980771	1.31977187959052
O	0.10847744729483	0.91859686454064	1.95341570679652
O	-0.13986210677371	-1.34609386199071	1.84817082940298
H	-2.11046963721295	-1.91595276795602	3.58360878190714
H	-1.25902031815806	-1.40413424330133	5.05096486170635
H	-1.70236109563006	-0.20498446634279	3.82649352437743
H	0.72879460778325	-0.73357366088252	3.63716151447074
H	0.35524358747051	-2.46272012979265	3.45165928717955
H	0.44245435530395	0.84036774811039	-1.94747001946391
H	1.29925364227740	1.37505076851835	-0.45934083136547
H	1.59872914411644	-0.22144112676194	-1.12813425334228

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Free carbene/B3LYP/6-311G(d)/BSS/70 degrees Constrained Optimization

C	-0.02085257922252	-1.45492370695459	3.29250117600757
C	-1.36427497022993	-1.23172923567852	3.96466654727592
C	0.88200444700031	0.38415607463021	-0.96023235131907
C	-0.23485986115728	-0.01307791093845	-0.09566041294891
C	-0.02906307774198	-0.10813058975315	1.32700011439965
O	0.13980416455344	0.92284155138743	1.95969817862897
O	-0.12989774947146	-1.34179087293410	1.84709339258541
H	-2.11811065750253	-1.91317285106415	3.56304956300633
H	-1.27757790628479	-1.41266075023924	5.04055516969174
H	-1.70532571045062	-0.20535221679846	3.81878872381127
H	0.72602444120187	-0.74345010472165	3.64769471114196
H	0.34664229335468	-2.46941219375522	3.44908433322389
H	0.57190538265327	0.74127020604368	-1.94413768621342
H	1.52731706392400	1.12744691165156	-0.46998549535688
H	1.51800619237355	-0.50626093387536	-1.11484583193446

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Free carbene/B3LYP/6-311G(d)/BSS/80 degrees Constrained Optimization

C	-0.02147012945127	-1.45594160609706	3.29558645253466
C	-1.37442142823824	-1.23968551651675	3.95020633050156
C	0.92824602586807	0.22639808979847	-0.95572141807211

C	-0.22939777648846	0.03451117808376	-0.07434097482083
C	-0.00846667072507	-0.09329339257725	1.34043467105555
O	0.17160820731376	0.93365408276858	1.97674530144988
O	-0.11048081754012	-1.33088990807715	1.84867164301098
H	-2.12175083996088	-1.91872588657243	3.53269147956318
H	-1.30280153676734	-1.42876807765038	5.02577196366673
H	-1.71509004033153	-0.21262961623854	3.80776400686171
H	0.72014464401307	-0.74713306550463	3.66619660893107
H	0.34517174534305	-2.47126591583946	3.44829627449343
H	0.67475906694195	0.61983040744739	-1.94191919322272
H	1.71867333314597	0.83421547894871	-0.49213018270043
H	1.37215747887704	-0.77576985097325	-1.10298283125265

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Free carbene/B3LYP/6-311G(d)/BSS/90 degrees Constrained Optimization

C	-0.01236225084261	-1.46060855784605	3.29359920320770
C	-1.38305352139723	-1.28682984128429	3.92319929706218
C	0.94483315393841	0.09053380202409	-0.94464529800614
C	-0.21791687136293	0.08870090915956	-0.04919535257387
C	0.00633331411746	-0.06040874356437	1.36287900551924
O	0.17059737226165	0.95659874720736	2.01748604028924
O	-0.07412662962135	-1.31045712215349	1.84684668447452
H	-2.10594846324982	-1.97506135993706	3.47858502533192
H	-1.32933541803356	-1.49313686825236	4.99662953261637
H	-1.74472900858738	-0.26544456470419	3.79175941339888
H	0.70580507695684	-0.74289615533656	3.69160323497818
H	0.37398926289869	-2.47024122962278	3.43492326537425
H	0.74182178368233	0.48993432742384	-1.93997889742287
H	1.83786495852845	0.56561587488855	-0.51355715199969
H	1.20584475771105	-0.97822568400225	-1.06486387024993

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Free carbene/B3LYP/6-311G(d)/BSS/100 degrees Constrained Optimization

C	0.08506025859624	-1.21502175818856	3.38790152906145
C	-1.32873298260492	-1.37719242304394	3.91748566437490
C	0.91334615544859	-0.20147063589886	-0.97328299852789
C	-0.28682388511665	-0.18536393256267	-0.12892994509737
C	-0.12296789721395	-0.07643601097201	1.29864345801311
O	-0.27856635457714	1.00904343540517	1.82952996308435
O	0.10786677738958	-1.24191552124458	1.93274793032798
H	-1.78933435094699	-2.28761467373709	3.52643298173680
H	-1.31347955202924	-1.44289565911365	5.00977306610085
H	-1.94917148495223	-0.52344182041747	3.63856204614258
H	0.53719629491835	-0.28328577542244	3.72897325366381
H	0.72441165950200	-2.04999443994980	3.67557579384732
H	1.71261006018013	0.47454695764445	-0.63582846594382
H	1.32049031169291	-1.22248606373066	-0.84568514864199
H	0.71583517271330	-0.05490615876790	-2.03662899614211

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Free carbene/B3LYP/6-311G(d)/BSS/110 degrees Constrained Optimization

C	0.08984947930137	-1.23012092693470	3.37398296811148
C	-1.32555444660035	-1.38331150887374	3.90240598861174
C	0.84898010157550	-0.38270252670906	-0.97185713884021
C	-0.30550306193334	-0.11735632070942	-0.10546028127388
C	-0.10349460173544	-0.01381223065456	1.32249278198571
O	-0.21209327807856	1.05425361766301	1.89357882396652
O	0.10862599343110	-1.20824255874215	1.91931776824493
H	-1.80411391820786	-2.27188610415760	3.48353898381632
H	-1.30894126242161	-1.48474608218864	4.99191707161975
H	-1.93107890360412	-0.50968975018339	3.65354956392795
H	0.56045286972090	-0.31891434248780	3.74385158900614
H	0.71373482913975	-2.08636712589335	3.63190875902278
H	1.74507883487663	0.20201333755055	-0.71509546799872
H	1.11976715172186	-1.43352878215581	-0.75995562109961
H	0.63772342981416	-0.29549330652334	-2.03890565710090

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Free carbene/B3LYP/6-311G(d)/BSS/120 degrees Constrained Optimization

C	0.09251675991150	-1.25503541500147	3.36200961144758
C	-1.32774261490337	-1.38214408703720	3.88517497777632
C	0.75599839111080	-0.54826167158805	-0.96893396105391
C	-0.30700195220151	-0.06137420102807	-0.08206994382887
C	-0.07635119904291	0.03008735211945	1.34715956735709
O	-0.15164885604226	1.07714744867728	1.95729982631418
O	0.11516408923525	-1.19008529175732	1.90979106984809
H	-1.83160500405672	-2.24376108836910	3.44037100568551
H	-1.31548931033507	-1.51581752535337	4.97124349326981
H	-1.90747397535695	-0.48435287661463	3.66224488672428
H	0.58932320982815	-0.36968128275285	3.75927494456468
H	0.68996914742121	-2.13694315626781	3.59531914428371
H	1.71498321756332	-0.02815554561924	-0.81812918057060
H	0.94790664644581	-1.59268517377552	-0.66726465327641
H	0.49465967842274	-0.53092208163210	-2.02822065654148

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Free carbene/B3LYP/6-311G(d)/BSS/130 degrees Constrained Optimization

C	0.09107003241248	-1.28230223093281	3.35136440940062
C	-1.33198066672564	-1.37637744394533	3.87508537322294
C	0.64901711615361	-0.68932930610897	-0.96588293213126
C	-0.29650324258273	-0.01816825118898	-0.06657514415576
C	-0.05920479177585	0.05253521999270	1.36591365283066
O	-0.12252038855242	1.07980398995824	2.00889081760262
O	0.11693386902069	-1.18611069379175	1.90198670863993
H	-1.86311310130942	-2.21255941159605	3.41360653989952
H	-1.32092020404549	-1.53436510171182	4.95788265697075
H	-1.88378020251887	-0.45640021914715	3.67346790744500
H	0.61504338744958	-0.42163924378084	3.76777430283776
H	0.66031359530486	-2.18769312203665	3.56467845794024
H	1.65609428471239	-0.24457717738582	-0.91628623308300
H	0.77340840112230	-1.72133378361111	-0.59925009672391
H	0.32384853533450	-0.71330608871366	-2.00738628869608

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Free carbene/B3LYP/6-311G(d)/BSS/140 degrees Constrained Optimization

C	0.08510297482176	-1.30153342414056	3.34363327730432
C	-1.33734669827676	-1.37691611249610	3.87274088876910
C	0.52815621702760	-0.80588496192149	-0.96543764763448
C	-0.27141373031902	0.02395064835937	-0.05807440052947
C	-0.04707983219409	0.06792771239409	1.37966231817485
O	-0.10339943738748	1.08003433158377	2.04693808660187
O	0.10745751112737	-1.18420411935665	1.89679325536272
H	-1.88589716324266	-2.19643214117286	3.40171042918475
H	-1.32463155770614	-1.55094584243584	4.95304572275781
H	-1.87273968082848	-0.44399450897125	3.68717325984568
H	0.62602280318475	-0.45668128160464	3.77080270266882
H	0.63803393109576	-2.22050948514431	3.54176449919317
H	1.58081852892329	-0.47958437964590	-0.99223780382935
H	0.55196547690840	-1.83122760415546	-0.56515973306301
H	0.14632693686571	-0.82276170629218	-1.98808472280680

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Free carbene/B3LYP/6-311G(d)/BSS/150 degrees Constrained Optimization

C	0.07981977814387	-1.31444801083133	3.33895873078055
C	-1.34130578372750	-1.37993574182046	3.87346864141172
C	0.39266552432642	-0.89638914415971	-0.96767839654823
C	-0.24154416255639	0.05709233530731	-0.05250741906099
C	-0.04185993933706	0.07801189006507	1.39001116586617
O	-0.09971185225556	1.07864451144415	2.07471952602317
O	0.09794964821587	-1.18299309589954	1.89416876030034
H	-1.90032401134621	-2.18940066953813	3.39727166439325
H	-1.32640202671440	-1.56391611322289	4.95209663717588
H	-1.86743671321036	-0.43972480038870	3.69859491566177
H	0.63065975265710	-0.47924924500519	3.77264607033041
H	0.62368161509769	-2.24113587784844	3.52649612701228
H	1.48021992192923	-0.72914139279122	-1.03528424140305

H 0.27562711049015 -1.91137380758207 -0.55946699652151
H -0.02000631071286 -0.86101159272886 -1.97822505342176

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Free carbene/B3LYP/6-311G(d)/BSS/160 degrees Constrained Optimization

C 0.07597800379345 -1.32352925751137 3.33401050314522
C -1.34237417933320 -1.38429077824197 3.87668525603111
C 0.24547488666735 -0.96012899160044 -0.97013759579337
C -0.21453396459174 0.08327680985605 -0.04994251515911
C -0.04559983532185 0.08569284021654 1.39688346454366
O -0.11163108588395 1.07733909288625 2.09403917343081
O 0.08729673744885 -1.18108011863638 1.89072454078955
H -1.90917925688924 -2.18703257367998 3.39819763144884
H -1.32236449550853 -1.57612751264574 4.95386900895869
H -1.86342982474642 -0.43954237548048 3.71164034974365
H 0.63377476670742 -0.49462097784660 3.77122402734178
H 0.61524076033828 -2.25486878303881 3.51185001387194
H 1.34531100958882 -0.98400102711446 -1.03873049189723
H -0.04935590616831 -1.94340305617526 -0.57491396638536
H -0.15429066810092 -0.84366045498735 -1.98012926807019

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Free carbene/B3LYP/6-311G(d)/BSS/170 degrees Constrained Optimization

C 0.07509903283975 -1.33087751652622 3.32367427323114
C -1.33731249858356 -1.39081763017280 3.88166479057829
C 0.08388142765863 -0.99697267105709 -0.96793435610767
C -0.19180454630959 0.11420728107227 -0.05305629042507
C -0.05486037953840 0.09650405299659 1.40033192966616
O -0.12468789458514 1.07949955674192 2.10790113188631
O 0.07137185882634 -1.17525216657682 1.88165893133843
H -1.91240974196033 -2.18770155902439 3.40319331145487
H -1.30625249851143 -1.59148709213241 4.95696961748625
H -1.85619765273665 -0.44268389135673 3.73003653107275
H 0.64051861026384 -0.50758970495866 3.76207918664062
H 0.61266974936518 -2.26579180012862 3.48739956125607
H 1.15466274255390 -1.25721982403846 -0.97956987509189
H -0.43914385143443 -1.89805382846732 -0.61479475662024
H -0.22646438684810 -0.78688015937126 -1.99428385436602

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Free carbene/B3LYP/6-311G(d)/BSS/180 degrees Constrained Optimization

C -0.00256784269465 -1.38367440071278 3.38152857233048
C -1.41053825535477 -1.32408912798864 3.95152340156607
C 0.01064017129115 -0.99067921162604 -1.07231886592217
C -0.01201133447643 -0.00889955257587 0.00456526237304
C -0.02526939964525 0.00486475516798 1.42841535660815
O -0.04467426860642 1.01024173613617 2.11848212047814
O -0.00584069247969 -1.26923636859936 1.93824863331774
H -2.04728284218681 -2.08753894184455 3.49701079245074
H -1.38524500747711 -1.49975260653842 5.03157374704436
H -1.85763331528913 -0.34379913021562 3.77789147317481
H 0.62415892863912 -0.59236077614116 3.79584650975733
H 0.46656223030388 -2.35042243687129 3.57090731601436
H 0.91375893121157 -0.89573039586413 -1.69002214503193
H -0.01555336452378 -2.00919116152064 -0.65936077688586
H -0.84586683371168 -0.87358558880565 -1.74902126527526

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Free carbene/B3LYP/6-311G(d)/BSS/190 degrees Constrained Optimization

C -0.05274540880157 -1.40860014914673 3.31911211320418
C -1.46705838078841 -1.30085524668119 3.86446782195401
C 0.05137057168081 -1.00212802362065 -0.96472878066763
C 0.24905847537103 0.10272584205963 -0.02243066702616
C 0.05571150743156 0.05453505783409 1.42279144349680
O 0.06056218778261 1.02690231980955 2.14878034508152
O -0.02412846366564 -1.22978510324789 1.88057007066663
H -2.13183859534290 -2.01127770111642 3.36634129947014
H -1.47150289205971 -1.52416700411472 4.93582994652737

H	-1.86051901615400	-0.29249103776162	3.72595383122653
H	0.60464416548336	-0.66703702891138	3.77594468145649
H	0.36322628067457	-2.40523968250716	3.47333504798677
H	0.38595513522637	-0.76053467045892	-1.97637546162738
H	0.60468176446079	-1.88356344726961	-0.60804031500194
H	-1.00478022629884	-1.31233733286698	-1.01628124474731

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Free carbene/B3LYP/6-311G(d)/BSS/200 degrees Constrained Optimization

C	-0.02924261075029	-1.37970613435501	3.34024573762503
C	-1.46047088749156	-1.32515064301824	3.84820239397599
C	0.03277832048332	-1.00390477579529	-0.96320425118928
C	0.3409905428345	0.06944733880348	-0.01443564655199
C	0.07212348816021	0.04584963301801	1.41640623793345
O	0.00626105650646	1.03318805223992	2.11993016551011
O	0.02682088120368	-1.23150564726597	1.89932606242019
H	-2.07956054219434	-2.07582813557035	3.35020949210887
H	-1.48291582546181	-1.52441086614223	4.92407856164477
H	-1.89484538095795	-0.33900131891079	3.67611050752540
H	0.58114036372845	-0.59802407508433	3.79567641320322
H	0.42841962155158	-2.35196127240265	3.52832889819933
H	0.47707621166939	-0.84265871066131	-1.94801869228340
H	0.39801197632958	-1.95716739029364	-0.55330171380779
H	-1.05395862206015	-1.13301926256161	-1.09428403431389

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Free carbene/B3LYP/6-311G(d)/BSS/210 degrees Constrained Optimization

C	-0.01086288127046	-1.35191504442816	3.36272409378681
C	-1.45702853132565	-1.34745855447231	3.82914385994880
C	0.01232030112177	-1.00245242596017	-0.95869416326106
C	0.43972082393038	0.02720501230155	-0.00676839144312
C	0.10077943616845	0.02965534941961	1.40861169452307
O	-0.02807694316182	1.03220866011535	2.08118979705372
O	0.07903539806021	-1.23624355617930	1.92023287499483
H	-2.02886609380157	-2.13646593314768	3.33389707042967
H	-1.50214074124451	-1.52061312601780	4.90882220393872
H	-1.92783227787338	-0.38564667242044	3.61915247304233
H	0.55179437096429	-0.53301254549089	3.81422721368626
H	0.48315623724113	-2.29805744229154	3.58808373452209
H	0.49957754260499	-0.91676284332831	-1.93221226592605
H	0.22959884537334	-1.99099545710316	-0.52690340854339
H	-1.07853838178716	-0.98329862899673	-1.11623665475266

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Free carbene/B3LYP/6-311G(d)/BSS/220 degrees Constrained Optimization

C	0.00357464972174	-1.32597926924148	3.38824301466875
C	-1.45451914809279	-1.36708908945394	3.81324748863220
C	-0.00830711052031	-0.99529376183624	-0.95774957423000
C	0.53597007504309	-0.02958375401265	0.00253207454755
C	0.13405045537218	0.00261140605184	1.39987289804635
O	-0.05260404657136	1.02176730700684	2.03241277468766
O	0.12974081772726	-1.24748893510087	1.94518412284314
H	-1.97991405491592	-2.19245546217601	3.32587450064503
H	-1.52427387905057	-1.51109452193050	4.89590936853971
H	-1.95672962108677	-0.43151043913483	3.56149657653019
H	0.51962749720050	-0.47204439567635	3.83029127451242
H	0.52867679622096	-2.24415490388428	3.65488797419961
H	0.48491502457725	-0.96579741827724	-1.93116643156860
H	0.09315946411804	-2.00290325983337	-0.52541216736968
H	-1.09072981474328	-0.85283671050090	-1.11035376268432

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Free carbene/B3LYP/6-311G(d)/BSS/230 degrees Constrained Optimization

C	0.01487652179682	-1.30280693925980	3.41731781977023
C	-1.45234613708814	-1.38094648926526	3.80296985512381
C	-0.02881415830629	-0.98140905234616	-0.96324977442018
C	0.62084797523121	-0.09899780313917	0.01256756627093
C	0.16749232449907	-0.03803941832258	1.39087235293637

O	-0.07469801337842	0.99888755892495	1.97402045839340
O	0.17939526809136	-1.26692348159523	1.97533478006801
H	-1.93555971724081	-2.23903246804330	3.32864405242091
H	-1.54829421248653	-1.49285860694491	4.88741572384075
H	-1.97827057616194	-0.47171524932401	3.50691544285254
H	0.48905448864555	-0.41743142678778	3.84395088586391
H	0.56348575142675	-2.19271392182119	3.72839471942388
H	0.44200498814910	-0.97113918926494	-1.94771210072431
H	0.00453609290473	-2.00442215622515	-0.55404830180790
H	-1.10107349108243	-0.75430456458547	-1.07812334801233

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Free carbene/B3LYP/6-311G(d)/BSS/240 degrees Constrained Optimization

C	0.07436465103431	-1.25323074563021	3.46606824555779
C	-1.38171069559675	-1.48924773774851	3.82782054826730
C	-0.11803302272114	-0.95947712111801	-0.96945048077692
C	0.57061839216057	-0.11787495104644	0.02127721917631
C	0.12441586771334	-0.05129679515778	1.39780678175475
O	-0.23446647206994	0.98021161664728	1.92963117040882
O	0.26318327896268	-1.24507521818378	2.02515575318853
H	-1.75183606397750	-2.41291057155706	3.37558368346040
H	-1.48820974132951	-1.57418099073268	4.91375402964765
H	-2.00300767846632	-0.65801519377171	3.48976630678110
H	0.43468040601260	-0.30605245498769	3.87032234467378
H	0.71572846329718	-2.06292767153935	3.81593152875597
H	0.62636336064240	-1.52248054649136	-1.54666314872954
H	-0.88092598930195	-1.64455675271382	-0.57945671181105
H	-0.58852765135995	-0.29673807396888	-1.71227713835487

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Free carbene/B3LYP/6-311G(d)/BSS/250 degrees Constrained Optimization

C	0.02712958564257	-1.27402565989866	3.48929384475098
C	-1.45705226466136	-1.39574702956125	3.78694599239884
C	-0.08865712115656	-0.91656988057324	-0.98642190270482
C	0.76603425765823	-0.28974344313707	0.02905969022252
C	0.27395241190937	-0.17258859480194	1.38231225187609
O	-0.01937582090048	0.91202823383827	1.84834429950551
O	0.28337692927027	-1.34214759242476	2.05965985744942
H	-1.86900875716093	-2.30959045012368	3.35113051629157
H	-1.61988718716550	-1.43137195055864	4.86857326744554
H	-2.00317677969593	-0.53848583270876	3.38908971303561
H	0.43382385627668	-0.33679318538752	3.87146614653271
H	0.59369060525743	-2.10911954483239	3.90262890650550
H	0.29288491391108	-0.83500603338580	-2.00546593695116
H	-0.11306022184184	-1.98734655388875	-0.71210775438773
H	-1.13803730234300	-0.58734569055584	-0.94923875997056

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Free carbene/B3LYP/6-311G(d)/BSS/260 degrees Constrained Optimization

C	0.03371361194379	-1.24863213488625	3.53144085912521
C	-1.45488680197951	-1.40156291922001	3.78964933005921
C	-0.10707775935696	-0.88933889815038	-1.00571360101729
C	0.80692403419038	-0.39929724474095	0.03309658988965
C	0.30700246597966	-0.25861892052207	1.37654513389002
O	-0.02108176281740	0.84666245554204	1.77096666473006
O	0.33891896183905	-1.38386243497088	2.11543619785083
H	-1.82521836779950	-2.34886410233359	3.38941585120710
H	-1.65072472660905	-1.38753321867875	4.86625325474273
H	-2.01407379698941	-0.58335895955061	3.33200102156619
H	0.40081735143247	-0.28110831828363	3.87582002507603
H	0.61120285074466	-2.04309856105717	4.00499922903300
H	0.26388441281600	-0.76623424119834	-2.02461676257895
H	-0.19633806620425	-1.97430646338294	-0.80800917023209
H	-1.13042530218994	-0.49469924656647	-0.92201449134167

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Free carbene/B3LYP/6-311G(d)/BSS/270 degrees Constrained Optimization

C	0.04213445322846	-1.22203829544614	3.56966209264624
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C	-1.44616887983770	-1.41297672670033	3.80301757775841
C	-0.11910438206273	-0.86344297084022	-1.03104560176302
C	0.82688891673757	-0.51333493910148	0.03560937756183
C	0.32149231031058	-0.34377143263827	1.37037963925005
O	-0.04381064143643	0.77414765864552	1.69681852505263
O	0.38670800861391	-1.42085933708219	2.16986421490658
H	-1.77491775064639	-2.39179443061629	3.44455192439124
H	-1.66769566799467	-1.35064898257244	4.87286622542644
H	-2.02225772265296	-0.63932053859239	3.29184092949470
H	0.36958078103907	-0.22646538129957	3.87091663778199
H	0.63414716053582	-1.97080598913517	4.09652024667149
H	0.27078935827783	-0.71764522272836	-2.03991973056753
H	-0.31851757911735	-1.94395975355942	-0.90194410243097
H	-1.09663125999501	-0.37093686633325	-0.92386782418006

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Free carbene/B3LYP/6-311G(d)/BSS/280 degrees Constrained Optimization

C	0.05165636838845	-1.19388149958259	3.59990031797836
C	-1.43141941482533	-1.43689702776507	3.81899217553185
C	-0.12496617949542	-0.84338370718873	-1.05724283047978
C	0.82773737766509	-0.62299927979399	0.03753402113930
C	0.31992619081497	-0.40679254699092	1.36557006449917
O	-0.08753962153500	0.71148976009205	1.63909440416993
O	0.42901110197826	-1.43879244308048	2.21658738494459
H	-1.71309489109303	-2.44331931497882	3.49888847587594
H	-1.67326819821723	-1.33793615400346	4.88162784526107
H	-2.03104901902126	-0.71127651730869	3.26604269919371
H	0.33327445951216	-0.17388902852365	3.86306277715539
H	0.66420085739516	-1.89428936639714	4.16815840001497
H	0.30645428476428	-0.72731509304237	-2.05297117132650
H	-0.48890627477688	-1.88328324604949	-0.96591620936981
H	-1.01937993655420	-0.21128774338666	-0.95405822258818

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Free carbene/B3LYP/6-311G(d)/BSS/290 degrees Constrained Optimization

C	0.06122811723076	-1.16987397337503	3.62453116043017
C	-1.41387248447155	-1.46108710752952	3.84035804789001
C	-0.12811121009424	-0.82338278512440	-1.08645874040250
C	0.80759183084995	-0.72603515964784	0.03951474178266
C	0.30192568051321	-0.45763061218234	1.36219206503646
O	-0.14914783986182	0.65227124581918	1.59825001726172
O	0.46184806909514	-1.44774369184921	2.25502767797907
H	-1.65437335489070	-2.48792225025816	3.55319105845655
H	-1.66918235687008	-1.33486011023594	4.89691211463685
H	-2.03565362924049	-0.77833715709999	3.25804286595133
H	0.30222786822449	-0.13178519991458	3.85513728583181
H	0.69361861955897	-1.82718226704383	4.22179932585323
H	0.34791197191390	-0.74045121659064	-2.06511867972695
H	-0.63398783155145	-1.80424056096660	-1.03761926577569
H	-0.92938634540609	-0.07559236200110	-0.99048954320471

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Free carbene/B3LYP/6-311G(d)/BSS/300 degrees Constrained Optimization

C	0.07009321269842	-1.15061647783415	3.64386274719793
C	-1.39502205788011	-1.48521946399636	3.86667619616126
C	-0.13026238631229	-0.79814158054699	-1.11707557908961
C	0.76998015377251	-0.82220368224772	0.04044571667450
C	0.27330621166735	-0.50092198185805	1.35908221211300
O	-0.21582862947450	0.59731936570170	1.57032146316637
O	0.48381801158033	-1.45301355408878	2.28454123223216
H	-1.59997948618930	-2.52735341648189	3.60862668465724
H	-1.65644945085370	-1.33754185365339	4.91892269045200
H	-2.03869790975193	-0.84079684983787	3.26481617767268
H	0.27537745070095	-0.09896175243258	3.84591227564422
H	0.72259958043415	-1.76935090119697	4.26040062343138
H	0.39022308797748	-0.73572658664462	-2.07468951547710
H	-0.73743833093398	-1.72035400089363	-1.12451585576898
H	-0.84908235243537	0.02902952801129	-1.02205693706704

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Free carbene/B3LYP/6-311G(d)/BSS/310 degrees Constrained Optimization

C	0.07397853537421	-1.14845301203038	3.65762831031493
C	-1.39056770581989	-1.47538738603964	3.89683106869541
C	-0.12569761143483	-0.78296442879245	-1.14697760030417
C	0.72030456169880	-0.94994037700934	0.03878836758078
C	0.25162320058837	-0.55980335237271	1.35379441814532
O	-0.23560410372947	0.54189609871132	1.54773395887681
O	0.48030754756847	-1.48442817373201	2.30503834598893
H	-1.59804630859801	-2.52327948764036	3.66562972077910
H	-1.64585076876221	-1.30134779934007	4.94653236503244
H	-2.03679986709895	-0.84505758945579	3.28293140968925
H	0.28141561739775	-0.09232466542975	3.83282071882587
H	0.72876771663122	-1.75297700030715	4.28576661982814
H	0.43500319330336	-0.78873931385236	-2.08390242920928
H	-0.86869053172570	-1.59749665913896	-1.19592230815654
H	-0.70750637039310	0.14644993842963	-1.06142283408699

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Free carbene/B3LYP/6-311G(d)/BSS/320 degrees Constrained Optimization

C	0.07727040598856	-1.13308676605875	3.66852046214034
C	-1.37798526927474	-1.48100152318550	3.93505196770161
C	-0.11309829748453	-0.76649810123768	-1.17964561692970
C	0.65476299022599	-1.04576175988644	0.03719212900113
C	0.20703564365339	-0.60529196515893	1.34676977688623
O	-0.302282323184798	0.48892986408163	1.52409547490448
O	0.47350849906818	-1.49701703336889	2.32152726076775
H	-1.56788064880608	-2.53844145657177	3.73432465453606
H	-1.62356717064682	-1.28372570573329	4.98294098536104
H	-2.04370014685208	-0.87970276506490	3.31295560169198
H	0.26608368389157	-0.06881599826576	3.81375911315844
H	0.75056030849391	-1.70844527655956	4.30453441486381
H	0.49059134212949	-0.81488280795741	-2.08865444554663
H	-0.93205451546446	-1.49785857910992	-1.28693065849492
H	-0.59660648807441	0.21774666607715	-1.10117098804164

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Free carbene/B3LYP/6-311G(d)/BSS/330 degrees Constrained Optimization

C	0.07934014066307	-1.11806566307006	3.67492194641103
C	-1.36287321952465	-1.49079967488436	3.97770315166028
C	-0.09530017953186	-0.74788944788308	-1.21210082238674
C	0.57888071951587	-1.12636634483178	0.03305020629192
C	0.15068636009791	-0.64852952410261	1.33852773951876
O	-0.38700460224106	0.43438790141388	1.50182413795757
O	0.45867934094945	-1.50717935858519	2.33117097781252
H	-1.53253240632945	-2.55682714585014	3.80655134906751
H	-1.59317139046026	-1.27272984674355	5.02493057787764
H	-2.05316539344161	-0.92001945033358	3.35377046620565
H	0.24651692654721	-0.04643827023649	3.79084902505754
H	0.77635655553053	-1.66254129696427	4.31263875201663
H	0.54382860275821	-0.85964322131092	-2.09126457016555
H	-0.98633623594625	-1.37747657328899	-1.37237900365349
H	-0.46126811358710	0.28626470867110	-1.14492380167129

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Free carbene/B3LYP/6-311G(d)/BSS/340 degrees Constrained Optimization

C	0.07889866024673	-1.10087878966295	3.6766626861416
C	-1.34510749319018	-1.50747518119190	4.02035916676518
C	-0.07324601495280	-0.72785822489583	-1.24088466230399
C	0.49705541721495	-1.19154883224480	0.02726323324390
C	0.08717695499147	-0.68625278326058	1.32919970199027
O	-0.48476938401497	0.38074356171361	1.48125158729063
O	0.44004387765120	-1.51204776489296	2.33520149957345
H	-1.48668580629957	-2.58189985767254	3.87879848414425
H	-1.55913292372580	-1.26999301959059	5.06684330709461
H	-2.06507226238734	-0.97278172158911	3.39806975085509
H	0.21639509037001	-0.02217338074119	3.76405534504687

H	0.80481070144431	-1.60912226679950	4.31215065494492
H	0.58280503103398	-0.92482868862320	-2.09263114086614
H	-1.03143933385075	-1.23415631764173	-1.44254607966525
H	-0.29909540953125	0.34642005909326	-1.18852698472796

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Free carbene/B3LYP/6-311G(d)/BSS/350 degrees Constrained Optimization

C	0.07014929858434	-1.06845878532360	3.67442700414822
C	-1.32232796795476	-1.54479435284935	4.05551842488074
C	-0.04309345748844	-0.70584401231151	-1.25873104660741
C	0.43314296966700	-1.24338831023120	0.01992433842098
C	0.01902143808280	-0.72122109431719	1.31704984226457
O	-0.61544752401945	0.31205335054751	1.45000484019217
O	0.43034369281542	-1.49815745255265	2.33859721651844
H	-1.40450240642936	-2.62919875202799	3.94763513042951
H	-1.53243467829694	-1.28861765577036	5.09839096270641
H	-2.08155020084777	-1.07052362698259	3.43095243141650
H	0.14671424937391	0.01857827900145	3.72826780086379
H	0.83466718490112	-1.51576788496449	4.31041572456554
H	0.53688994061546	-1.07376855754658	-2.10853677661347
H	-1.09718746641996	-0.97801959283685	-1.42880600320973
H	-0.01174796758334	0.39327524016537	-1.24983975797626

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Free carbene/BP86/6-311G(d)/Triplet state/0 degrees Constrained Optimization

C	0.00683468284037	-1.36730649747254	3.39348127748792
C	-1.41322917660622	-1.30876957657146	3.94059564266085
C	-0.00213035442585	0.98475897103680	-1.04171726624632
C	0.00845589396509	-0.09063924606894	-0.04717755082926
C	-0.00762416687084	-0.06481891174597	1.38927828422610
O	-0.03550416768111	0.98341756294857	2.04030621723949
O	0.01870898896267	-1.31523849917702	1.93694245966527
H	-2.03583587652955	-2.10365704572011	3.50263952712511
H	-1.40196900942737	-1.44478528652968	5.03431304468491
H	-1.87587599319995	-0.33562790240464	3.72298992598354
H	0.61972385359274	-0.54102155692277	3.78302071931952
H	0.49396597523065	-2.32453875431613	3.62650977958264
H	-0.90486723353286	0.94033242053191	-1.67920586125065
H	0.02170706166906	1.97637347853082	-0.55314406269889
H	0.86533029701316	0.91657478988118	-1.72356200395022

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Free carbene/BP86/6-311G(d)/Triplet state/10 degrees Constrained Optimization

C	-0.01366404661467	-1.45275187022518	3.34306389797978
C	-1.37381722599111	-1.22160224705865	3.98792392808597
C	0.11217629766680	0.98728274239490	-1.03492896868057
C	-0.10818753333823	-0.08943632019445	-0.06578344459271
C	0.00995564165321	-0.10897583952404	1.36634915802037
O	0.16895766835514	0.91734293268401	2.03343777803938
O	-0.09234731273782	-1.36492864211019	1.88999559556487
H	-2.12431034659539	-1.91642315489797	3.58146252237460
H	-1.30783971627722	-1.38528143669206	5.07590427369215
H	-1.71669332229952	-0.19093622488557	3.81876584850306
H	0.72852559286226	-0.72494867407029	3.70284707525367
H	0.35605280052713	-2.47148249948843	3.52552340974128
H	-0.29140783723552	0.72984480344480	-2.02790971780476
H	-0.35680873637979	1.93495831885192	-0.70685352639249
H	1.19360686540473	1.19051472477120	-1.16452769678462

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Free carbene/BP86/6-311G(d)/Triplet state/20 degrees Constrained Optimization

C	-0.00662758100072	-1.44193339529477	3.35916594422488
C	-1.38933687036374	-1.24462752615085	3.96606646152467
C	0.27991766842806	0.94619296471347	-1.04011178188056
C	-0.07687106083696	-0.06690947746398	-0.04415414701371
C	0.03604822394097	-0.08682406790573	1.38944612958026
O	0.15217269169671	0.93784235759850	2.06681830404808
O	-0.04652474554034	-1.34855046077224	1.90461310039541

H	-2.11198379018864	-1.95448026923080	3.53580417830878
H	-1.35053207142301	-1.41152639309920	5.05487973796953
H	-1.75093972665403	-0.22132983308800	3.79130387221474
H	0.70870062966848	-0.69973580911558	3.74294093765171
H	0.38078567066892	-2.45302439113627	3.54722976954095
H	-0.31559419550692	0.83968113833200	-1.96265055691411
H	0.13286148144622	1.97191978601436	-0.65121306393370
H	1.34359259666501	0.85217502259909	-1.33486875271694

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Free carbene/BP86/6-311G(d)/Triplet state/30 degrees Constrained Optimization

C	-0.00805505036316	-1.44942801191214	3.36477888336810
C	-1.39641941740074	-1.25097190493532	3.95815040587238
C	0.43261349556572	0.88051436222335	-1.04850504121872
C	-0.06460206839801	-0.04051348745400	-0.02454992586247
C	0.06094366116923	-0.07327543100394	1.40914095957715
O	0.17653940975114	0.94184424939122	2.09966468245606
O	-0.03212098925584	-1.34030669240194	1.91047779846876
H	-2.11784633237474	-1.95280745042253	3.51297562656872
H	-1.37049009988321	-1.42859222846455	5.04566409857275
H	-1.75093865868359	-0.22416027984122	3.78955064308410
H	0.70693939261100	-0.71522674765295	3.76400978667535
H	0.37195338675064	-2.46456109162222	3.54593116134895
H	-0.19760618322845	0.86389783086703	-1.95419975132068
H	0.47180721724341	1.92390648563993	-0.67999811191387
H	1.45503114249660	0.59832505458927	-1.36782108267658

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Free carbene/BP86/6-311G(d)/Triplet state/40 degrees Constrained Optimization

C	-0.01348502919285	-1.46175996724075	3.36824742020437
C	-1.40373252203452	-1.25504698085697	3.95421758408334
C	0.57277539066747	0.79021580736559	-1.06026710564874
C	-0.04805886346704	-0.00828064029218	-0.00256353127616
C	0.08484614545689	-0.05873999891517	1.43162057162949
O	0.20736503645079	0.94313337731759	2.13850661355999
O	-0.02637209178310	-1.33198124669137	1.91491811546530
H	-2.13002995152282	-1.94229756152201	3.49447435084500
H	-1.38780306167265	-1.44744702991906	5.03940770837188
H	-1.74501446109243	-0.22197130280297	3.79698051893298
H	0.70717033652489	-0.74161707937034	3.78242871493445
H	0.35329644481875	-2.48376968881619	3.53755045571765
H	-0.05753738351144	0.82876612475209	-1.96541636700974
H	0.76189541485316	1.83315794297373	-0.73784057148747
H	1.54227176950489	0.35078129701802	-1.36699434532233

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Free carbene/BP86/6-311G(d)/Triplet state/50 degrees Constrained Optimization

C	-0.02199699374854	-1.47418567980926	3.37197725554442
C	-1.41368090623280	-1.25870283657556	3.95127686555410
C	0.69852902678206	0.67569887883035	-1.07449583308622
C	-0.02004651636450	0.02621160817524	0.02126670581989
C	0.10789111129622	-0.04226941979308	1.45679143391126
O	0.23646292679472	0.94485303761206	2.18126777632724
O	-0.02341969685896	-1.32187695959210	1.92025752454036
H	-2.14532418046757	-1.92953448887646	3.47602868646947
H	-1.40790589621809	-1.46775051328769	5.03349194010891
H	-1.74064173019143	-0.21906688782176	3.80749485564680
H	0.70463880996528	-0.76950996767287	3.80191837517163
H	0.33066126783677	-2.50329312617489	3.52782905952436
H	0.07461501015517	0.74734232768306	-1.98220510045971
H	1.02419298347700	1.70278598620199	-0.81380989212709
H	1.6005519677467	0.09611075210097	-1.35381952094545

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Free carbene/BP86/6-311G(d)/Triplet state/60 degrees Constrained Optimization

C	-0.03378668733608	-1.48510408934190	3.37726078608022
C	-1.42754690353446	-1.26114897451469	3.94811570844460
C	0.80645796382719	0.53890791951824	-1.09044750554282

C	0.02537531754763	0.05947598516889	0.04717623675123
C	0.13242181338152	-0.02545722247037	1.48412426206647
O	0.26447049846603	0.94699828254948	2.22585645845468
O	-0.02127441311184	-1.31111716261359	1.92760636362437
H	-2.16327740769028	-1.91607190058886	3.45722359955478
H	-1.43364968357952	-1.48545086236747	5.02726703436493
H	-1.74059238024920	-0.21563522370995	3.81646965335732
H	0.69754870903999	-0.79548833244712	3.82336998716464
H	0.30522659355459	-2.52062861215821	3.52070084133651
H	0.18238277809778	0.63084200688725	-1.99644541474345
H	1.26181525379518	1.53309983293317	-0.90465226482728
H	1.62516361179148	-0.16575266684489	-1.33835561408620

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Free carbene/BP86/6-311G(d)/Triplet state/70 degrees Constrained Optimization

C	-0.04583493326770	-1.49341767987462	3.38437438179537
C	-1.44231272288814	-1.26148769433855	3.94495602155236
C	0.89144241765531	0.38593863689985	-1.10481973982162
C	0.07996102782889	0.08019599314558	0.06887799311280
C	0.15315453529784	-0.01575711745213	1.50655202327511
O	0.28367738741498	0.94639527140362	2.26061778240562
O	-0.01862346261168	-1.30547570898471	1.93610616983378
H	-2.17993932753447	-1.90444444778538	3.44123997305980
H	-1.46032634518336	-1.49619692142720	5.02177120976991
H	-1.74379470137074	-0.21171005288789	3.82067150897041
H	0.68806064844034	-0.81489452520313	3.84309968923742
H	0.28204394436674	-2.53354940723614	3.52050909081233
H	0.26256351801350	0.50085566981134	-2.00519319896985
H	1.46876021733440	1.32650179322768	-0.99116922884390
H	1.61290926950409	-0.42720043229831	-1.32232354418953

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Free carbene/BP86/6-311G(d)/Triplet state/80 degrees Constrained Optimization

C	-0.05748469213292	-1.49964568484136	3.39212750462611
C	-1.45662148651653	-1.26069817467513	3.94305020260650
C	0.94937839868328	0.22300044326438	-1.11719505600691
C	0.13559787796769	0.08554299036865	0.08473111792153
C	0.16958431092120	-0.01398077389413	1.52193988793346
O	0.29756508708003	0.94288425516585	2.28226575400181
O	-0.01770434196285	-1.30557021456336	1.94491484207588
H	-2.19475349961752	-1.89649539379687	3.43104370356679
H	-1.48444333015275	-1.49977599876188	5.01871064982064
H	-1.74973792221510	-0.20833727118171	3.82077563498456
H	0.67711564346247	-0.82773512625436	3.85945975253677
H	0.26240599066418	-2.54256575899714	3.52644187594268
H	0.31530527714508	0.36520586103736	-2.01025533566035
H	1.63587139684088	1.09312655828390	-1.06879276343180
H	1.56480255183286	-0.68044931015422	-1.30394763891766

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Free carbene/BP86/6-311G(d)/Triplet state/90 degrees Constrained Optimization

C	0.00065317428992	-1.37787063346620	3.46785648183110
C	-1.44942320683186	-1.33793376401004	3.93056227265858
C	0.97044200570842	0.01114515445655	-1.14839975192412
C	0.15428758102829	-0.02122531647132	0.05910685902751
C	0.09170547224390	-0.01384698983192	1.49452001199252
O	0.01028138946616	1.00198188391212	2.18156600026059
O	0.09646542890072	-1.28620522227031	2.01333233200063
H	-2.04126368854492	-2.12346974421909	3.43668502864903
H	-1.50271189954350	-1.50109108222751	5.01937496569675
H	-1.90230593679726	-0.36100213315697	3.70995888753495
H	0.58534698118374	-0.55960552118560	3.91305001491777
H	0.47825972159595	-2.33960663298984	3.70266814438701
H	0.80741562813011	0.92763807032305	-1.74783305065194
H	2.04826146960054	-0.01986434152336	-0.89333095238254
H	0.77220339656979	-0.85097019333957	-1.81384711199785

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Free carbene/BP86/6-311G(d)/Triplet state/100 degrees Constrained Optimization

C	0.03944864359145	-1.26144921691902	3.49330384321089
C	-1.40555669568553	-1.39426241034744	3.95426213760721
C	0.98278407910261	-0.19978418910289	-1.13981134470852
C	0.07456252090018	-0.12785442779720	-0.00194057818823
C	-0.03817837579399	-0.03524566411647	1.42993946124663
O	-0.26996005457531	1.00409394156510	2.04144042369319
O	0.13301444935265	-1.25733213070487	2.03575609378285
H	-1.87691127415720	-2.28817597088313	3.51832371466709
H	-1.44446608929584	-1.48609873817527	5.05203080555553
H	-1.98961481858590	-0.50889683957007	3.66571772354364
H	0.49925713994872	-0.33993374683292	3.87952076282081
H	0.64586409344480	-2.12755291306304	3.79404070805500
H	1.59817646048839	0.71737383753462	-1.23786848441378
H	1.67553463004059	-1.06378367000319	-1.07331149603421
H	0.42378547422438	-0.30953234158421	-2.08613363883809

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Free carbene/BP86/6-311G(d)/Triplet state/110 degrees Constrained Optimization

C	0.03781697592427	-1.27530875501977	3.46839653133197
C	-1.39433904014900	-1.38004053381477	3.97476077546965
C	0.94085982583615	-0.36716675151679	-1.13122559804789
C	0.02589807980677	-0.12424238441885	-0.02128957842647
C	-0.07409391046838	-0.03774166625177	1.41262416033693
O	-0.26492743613933	1.00433227584371	2.03254339254733
O	0.08541802801133	-1.26715801156572	2.00916836062619
H	-1.89759628447536	-2.26310298934292	3.55244329131017
H	-1.39994117696581	-1.47367398300893	5.07309713436093
H	-1.96897001904793	-0.48216963314027	3.70646928185057
H	0.52794937253932	-0.36461949899200	3.84320746778769
H	0.63557567746824	-2.15459115261138	3.74786376060697
H	1.67647118806147	0.45470918777984	-1.24141985503761
H	1.50782364210651	-1.31332582292217	-1.01223850079993
H	0.39548829449176	-0.43580489201820	-2.08913049191650

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Free carbene/BP86/6-311G(d)/Triplet state/120 degrees Constrained Optimization

C	0.03642942386076	-1.29115239050210	3.44023217064016
C	-1.38159621517828	-1.36804548334146	3.98921577430119
C	0.86689551385069	-0.52408556890799	-1.11733982672819
C	-0.02071828706541	-0.10526829476865	-0.03640405447157
C	-0.10606229069896	-0.03133493099742	1.39901514273756
O	-0.25565078542090	1.00900489169825	2.03252975533648
O	0.03974586981021	-1.27132069085462	1.98038176416407
H	-1.91762988056509	-2.23541819666298	3.57482673169284
H	-1.35611950320761	-1.47198638025488	5.08633059726157
H	-1.94312377482766	-0.45484016749495	3.74633922503847
H	0.55808511951722	-0.39464152732719	3.80654924916332
H	0.62253822859683	-2.18580111922710	3.69452454510480
H	1.71274113594173	0.18116837426512	-1.24056506152449
H	1.29210768128183	-1.53385363511633	-0.94548484403152
H	0.33556599210465	-0.55440947650769	-2.08488103668469

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Free carbene/BP86/6-311G(d)/Triplet state/130 degrees Constrained Optimization

C	0.03456009067784	-1.30625955358890	3.41662068794966
C	-1.37279256299488	-1.36238878297613	3.99494637178029
C	0.76362335810469	-0.66374427408835	-1.10474226219283
C	-0.05052020743275	-0.07797958197848	-0.04226228152113
C	-0.12144643232352	-0.01829778351708	1.39379542971621
O	-0.23558454874186	1.01775075144755	2.04174640377511
O	0.00789115407005	-1.26961074020175	1.95793950412305
H	-1.93410606240792	-2.21471020173612	3.58270980447823
H	-1.32606435211478	-1.47908978589366	5.09009661980180
H	-1.92145606846899	-0.43590742760813	3.77390046435558
H	0.58060988026680	-0.42384652361773	3.78179183526039
H	0.60869644779191	-2.21462091715001	3.64901243657999
H	1.70079993798793	-0.09131991484753	-1.25148687786491

H 1.04064763005706 -1.71454461869385 -0.88590565336586
H 0.23284835952840 -0.65725350954984 -2.07289235087559

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Free carbene/BP86/6-311G(d)/Triplet state/140 degrees Constrained Optimization

C 0.03273078779108 -1.31951819747951 3.40172725489683
C -1.36942868897182 -1.36096797726798 3.99379099961234
C 0.63543281550936 -0.78139974595984 -1.09617070653348
C -0.06413848828042 -0.05188517928500 -0.04020857553115
C -0.12030280704646 -0.00524927561623 1.39552164659170
O -0.20726166058803 1.02569756658788 2.05626789747398
O -0.00793407937693 -1.26674344615406 1.94434542137531
H -1.94769642667711 -2.20024194997010 3.57817867877827
H -1.31357576644037 -1.49031224474975 5.08709918556305
H -1.90620745389338 -0.42400246663532 3.78828858073058
H 0.59521843465096 -0.44895141090416 3.77035882396558
H 0.59576507628370 -2.23854779285377 3.61904877531662
H 1.64023390282444 -0.35206961157349 -1.27819344641005
H 0.76739694430152 -1.85105557229204 -0.83925410509350
H 0.09114368991344 -0.73351557084663 -2.05553029873608

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Free carbene/BP86/6-311G(d)/Triplet state/150 degrees Constrained Optimization

C 0.03058557807315 -1.33094497203641 3.39413637513474
C -1.37100264018721 -1.36169097082688 3.98838812504484
C 0.48783942557417 -0.87422948388598 -1.09130841563234
C -0.06649412010941 -0.03050705466425 -0.03367206410108
C -0.10699981657627 0.00505013568728 1.40133648199878
O -0.17341142444820 1.03140968681359 2.07229606350675
O -0.01172790313433 -1.26456379563612 1.93787347295416
H -1.95969408044273 -2.19042169361971 3.56622493221680
H -1.31489532206787 -1.50160116407891 5.08039182244782
H -1.89725440099235 -0.41673248725025 3.79235485844298
H 0.60329397620149 -0.46992370544096 3.76938438828225
H 0.58358613388700 -2.25812832815320 3.60260510468771
H 1.53424183776469 -0.59165940370140 -1.31932399850983
H 0.48377163113827 -1.94328135293820 -0.80213491694616
H -0.07980632368038 -0.77774616526859 -2.03328209752745

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Free carbene/BP86/6-311G(d)/Triplet state/160 degrees Constrained Optimization

C 0.02746913213550 -1.34150605677482 3.39136756153882
C -1.37688842221000 -1.36243673850700 3.97966216440971
C 0.32651626136960 -0.94026271448098 -1.08793767260790
C -0.06087398397808 -0.01379267378677 -0.02496359892170
C -0.08513156006774 0.01248297795860 1.40932571642811
O -0.13477125309178 1.03480207337355 2.08848249823621
O -0.00790956409977 -1.26367245511303 1.93589380826638
H -1.97234052324465 -2.18187313373467 3.54886939677337
H -1.32688168310455 -1.51113856824409 5.07078951773536
H -1.89267977842535 -0.41067022657994 3.78869201091356
H 0.60704556198149 -0.48896398964838 3.77522846862748
H 0.57026823675886 -2.27569532052355 3.59539761565259
H 1.38591944615672 -0.79762930297053 -1.37746600251013
H 0.20593304194297 -1.99272190181073 -0.76635905004551
H -0.27535796412322 -0.79289913315766 -2.00171230249635

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Free carbene/BP86/6-311G(d)/Triplet state/170 degrees Constrained Optimization

C -0.00113393787975 -1.37556488961961 3.39245609916813
C -1.41286640503562 -1.33844723050031 3.96116210357056
C 0.17739548592162 -0.97337230031862 -1.08396651980051
C -0.00055179527956 -0.00170261962851 -0.00617030873018
C -0.02022584540587 0.00770843510291 1.42748654871461
O -0.02267702752603 1.02232028898255 2.12012145440900
O -0.01188045293353 -1.27847798148756 1.93781451337237
H -2.03955866103501 -2.12447016748439 3.51267731185054
H -1.38570994490507 -1.50197847290992 5.05100808160913

H	-1.88229488398687	-0.36192475195049	3.77541089757355
H	0.61220765512148	-0.55561926639331	3.79439110542472
H	0.49527273461708	-2.33623359324137	3.59177337252137
H	1.08953658944641	-0.76480435204078	-1.67385588645026
H	0.25980649641809	-1.99973273271325	-0.67868865674897
H	-0.66825003653738	-0.95881731879733	-1.79634998448406

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Free carbene/BP86/6-311G(d)/Triplet state/180 degrees Constrained Optimization

C	-0.00132674797573	-1.37689631157461	3.39580283655062
C	-1.41845712925272	-1.33747119302153	3.95165678760510
C	0.00109403109662	-0.98797299003435	-1.08125305125351
C	0.00111438228631	-0.00119483847892	-0.00212513043930
C	-0.00073686973796	0.00641343398171	1.43122000888707
O	-0.00017410681754	1.02120376995904	2.12397243544984
O	0.00206882270629	-1.27976329418684	1.94144449466393
H	-2.04169500264698	-2.12415616551853	3.49961440505303
H	-1.40079897664517	-1.49796250652426	5.04209468740854
H	-1.88490616904407	-0.36085873772590	3.75904496127182
H	0.60911021929868	-0.55783518810695	3.80373772145050
H	0.49131923481986	-2.33843189440129	3.59992187718653
H	0.91461238921457	-0.91669292206826	-1.70083850878849
H	-0.05278763429998	-2.01507162772196	-0.67340360109176
H	-0.85579933800220	-0.84716274257734	-1.76561979195393

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Free carbene/BP86/6-311G(d)/Triplet state/190 degrees Constrained Optimization

C	0.02006812470595	-1.35355185047719	3.41493032114823
C	-1.41864315868854	-1.36208171228634	3.91359488395992
C	-0.03099613232813	-0.99028431442421	-1.06787969603421
C	0.07640305909511	-0.00454338366094	0.00671523678900
C	0.04769442095818	0.01495100646537	1.43977046511127
O	-0.00901162189391	1.03386103471205	2.12383997724258
O	0.07852493419531	-1.26709524573489	1.96059013069043
H	-1.99442635410462	-2.17462950982468	3.44461556295651
H	-1.43894847084679	-1.51353692242619	5.00530159872785
H	-1.91244141168028	-0.40476647698442	3.69396110885539
H	0.58364234901841	-0.50962051583016	3.83907401300973
H	0.53879901890023	-2.29488572202383	3.64661424457388
H	0.88776482643537	-1.03134989462048	-1.68271684718351
H	-0.20389862299169	-2.00235758551864	-0.65532694779490
H	-0.86189385577460	-0.75396211536545	-1.75781392005216

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Free carbene/BP86/6-311G(d)/Triplet state/200 degrees Constrained Optimization

C	0.00711138539524	-1.35384761726891	3.43928832299495
C	-1.45319210235694	-1.34444219711368	3.87102157586371
C	-0.03276905970822	-0.99653378523459	-1.05678277415931
C	0.21424370743776	-0.04121233943953	0.02223597927742
C	0.14144337397951	-0.00613151646520	1.45453617464068
O	0.07168851429283	1.02089742425620	2.12455381814171
O	0.13322844637629	-1.28187185007115	1.98867639868395
H	-2.01436584688315	-2.15593377906250	3.38288705761749
H	-1.52550397289506	-1.48544162844496	4.96185285006412
H	-1.92707993807052	-0.38468294824818	3.62003992040828
H	0.55855520507731	-0.51112424634753	3.88136192512629
H	0.50529615556593	-2.29758428283754	3.70392396989193
H	0.65288050296925	-0.84084426994944	-1.90830975404648
H	0.09234096322084	-2.03876860958988	-0.70529877715054
H	-1.06124022940106	-0.89633156218314	-1.45471655535421

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Free carbene/BP86/6-311G(d)/Triplet state/210 degrees Constrained Optimization

C	0.02013355411677	-1.33416390883710	3.46589484067570
C	-1.45411609334802	-1.35717076658462	3.84657177451932
C	-0.05600501331299	-0.99640280882426	-1.05631560855869
C	0.28922701664501	-0.08067209261201	0.02973963646172
C	0.18400611540835	-0.01986408463359	1.46063630808268

O	0.06532142666997	1.01669881041951	2.10799979886292
O	0.19563464591094	-1.28407923598592	2.01899489961386
H	-1.97590469081794	-2.19231812198970	3.35467525212801
H	-1.56094725644080	-1.48086853136278	4.93665945712381
H	-1.94462439874260	-0.41535966958346	3.56183820797567
H	0.53348224016637	-0.46936538876823	3.91107369383130
H	0.53361132688577	-2.25940350310593	3.76417258602843
H	0.60868495508911	-0.86732578454209	-1.92847490568490
H	0.01301020800130	-2.05338673801977	-0.73309301903613
H	-1.08887693123122	-0.82017138357007	-1.41510279002369

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Free carbene/BP86/6-311G(d)/Triplet state/220 degrees Constrained Optimization

C	0.03272320972647	-1.31532419801048	3.49535463733437
C	-1.45048511993412	-1.36985964308241	3.83548253165462
C	-0.07745747765389	-0.99082670372526	-1.06674040059225
C	0.35165947545054	-0.13346400482764	0.03625739087963
C	0.21413256136674	-0.04322583937310	1.46441390449388
O	0.04877468592123	1.00354505851568	2.08374823410980
O	0.24802217068764	-1.29183228857338	2.05242505972169
H	-1.93591320763279	-2.22923626949263	3.34809777348653
H	-1.58484047496095	-1.47323040032969	4.92464171742082
H	-1.95761496131130	-0.44796040754117	3.51675820916689
H	0.51083776426940	-0.42781766059416	3.93493103490277
H	0.56164213877088	-2.22001306833483	3.82753172157499
H	0.58434747342944	-0.88862051216414	-1.94463883969153
H	-0.08507301178141	-2.06029988709510	-0.77716277876343
H	-1.09811812134789	-0.72568738337171	-1.40583006369877

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Free carbene/BP86/6-311G(d)/Triplet state/230 degrees Constrained Optimization

C	0.04433130999860	-1.29914782699246	3.52628932958317
C	-1.44325200256290	-1.38239490184018	3.84022755454657
C	-0.09614632383169	-0.97823893429061	-1.08952005532956
C	0.40054319048425	-0.19879658369049	0.04172543817246
C	0.23053966018970	-0.07663927905906	1.46536264962468
O	0.02618344210318	0.98062663752803	2.05395587143402
O	0.28670348891231	-1.30668082405806	2.08688547539812
H	-1.89779894571020	-2.26551708014940	3.36564789173551
H	-1.59586871937752	-1.46237742371093	4.92894855843603
H	-1.96696258761921	-0.48172039209391	3.48925467711681
H	0.49239485408079	-0.38939904883932	3.95180261873568
H	0.58884514048818	-2.18194124738662	3.89052159650031
H	0.57516744931809	-0.89808746786482	-1.96260322381566
H	-0.19123920605129	-2.05509757655925	-0.84387832932189
H	-1.09080364542228	-0.61844125899292	-1.41934992081623

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Free carbene/BP86/6-311G(d)/Triplet state/240 degrees Constrained Optimization

C	0.05544622869883	-1.28826554956519	3.55822079759833
C	-1.43211608571181	-1.39398279862388	3.86519925010682
C	-0.11036881171489	-0.95584239761116	-1.12849119184755
C	0.42775245039650	-0.27659021886545	0.04626733878320
C	0.22802340088833	-0.12308477291911	1.46375063736266
O	-0.00595096658101	0.94513620651897	2.02038702569858
O	0.30760229503848	-1.33138274719540	2.12078654355365
H	-1.86485185557015	-2.29899495560162	3.41202207341928
H	-1.59028489487748	-1.44760080468025	4.95470591581264
H	-1.97208386582512	-0.51437007197094	3.48653122117152
H	0.48174773834586	-0.35781969884949	3.96068391807879
H	0.61563128435077	-2.14901722637661	3.95030730585710
H	0.58530792342140	-0.89008688715505	-1.98360368609735
H	-0.29874759315088	-2.03287333623919	-0.94259380787427
H	-1.06447014270880	-0.49907794886563	-1.45890320962338

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Free carbene/BP86/6-311G(d)/Triplet state/260 degrees Constrained Optimization

C	0.06294297161272	-1.26015650312447	3.61615469299910
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C	-1.41657843520965	-1.41252274268667	3.94216551672455
C	-0.09618427987832	-0.91263067863692	-1.22099423067828
C	0.43211222717038	-0.44297008744659	0.05361243487341
C	0.16862283843634	-0.22654574536980	1.45147230051765
O	-0.12155425848631	0.86092448622513	1.94279334632075
O	0.30811564958098	-1.38288801516929	2.18214805572004
H	-1.81079500940568	-2.36154318839746	3.54766289290039
H	-1.56566426564502	-1.40716148508586	5.03423837354787
H	-1.99739544749088	-0.58222784706703	3.51565291995928
H	0.44931601202362	-0.28820307616957	3.95637474410850
H	0.66332689170896	-2.06893373672797	4.05644490590439
H	0.68620577706197	-0.90264033530849	-2.00070664685304
H	-0.47643933450336	-1.95307829791612	-1.16117508263152
H	-0.92339423197574	-0.27327595511890	-1.59057409141307

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Free carbene/BP86/6-311G(d)/Triplet state/270 degrees Constrained Optimization

C	0.06712498617366	-1.24891265310602	3.63464010665851
C	-1.40743491480370	-1.42362597701443	3.97175830045864
C	-0.09105204900242	-0.88810933070528	-1.25185095591244
C	0.43550215887544	-0.51613939582274	0.05502121147445
C	0.14124614187896	-0.27448208562959	1.44280034417623
O	-0.17624456455067	0.81840650527218	1.90573339822780
O	0.30908191632988	-1.40595444026268	2.20343675591870
H	-1.78309008346277	-2.39080317325505	3.60423725934735
H	-1.55173464244846	-1.39261798237225	5.06402560376165
H	-2.00734588145813	-0.61725673444830	3.52630504787421
H	0.43404592340214	-0.26001923500807	3.94649896391986
H	0.68631899238951	-2.03252598620601	4.09389987912669
H	0.71213811751257	-0.90562691790392	-2.00993812579279
H	-0.54591825717869	-1.89972526298869	-1.24527706047251
H	-0.8600073865733	-0.17646053854916	-1.61602059676633

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Free carbene/BP86/6-311G(d)/Triplet state/280 degrees Constrained Optimization

C	0.07080997506016	-1.23700760845437	3.64876983395552
C	-1.39972028307032	-1.43537372614546	3.98987667100188
C	-0.08868241311235	-0.86260977941774	-1.26839770238269
C	0.45874310248459	-0.59021435004270	0.05524259300526
C	0.12583283367290	-0.32408329504159	1.43181560255861
O	-0.22457138407732	0.77231297241210	1.86267180484649
O	0.31865702098474	-1.42801318488266	2.22249877165086
H	-1.75319629808171	-2.42053005831844	3.64912703108744
H	-1.54548104220286	-1.37782129730656	5.08085553982758
H	-2.01691054499367	-0.65506045599361	3.52231353802887
H	0.41524337134840	-0.23186866132927	3.93330184875528
H	0.70673698346674	-1.99390801635055	4.12935504295074
H	0.71109080230543	-0.88767030718473	-2.02961632552785
H	-0.59651930341249	-1.84767497366222	-1.30770123100624
H	-0.81939571537225	-0.09433046628221	-1.59484288675174

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Free carbene/BP86/6-311G(d)/Triplet state/290 degrees Constrained Optimization

C	0.07527727429015	-1.22122610262351	3.66089400411732
C	-1.38966991541407	-1.45325184199212	4.00471567851907
C	-0.08809500453090	-0.83297796858559	-1.27884733816313
C	0.48303912999540	-0.67031440686265	0.05434613360225
C	0.11214080730818	-0.37821933485642	1.41751541445885
O	-0.27615656269145	0.71992086916377	1.81130004144246
O	0.33335648039434	-1.44960120842377	2.24208917578967
H	-1.71225620534579	-2.45851790788927	3.69335820708468
H	-1.54029328789679	-1.36705211906840	5.09314092034545
H	-2.02856072696497	-0.70649185259812	3.51221141925528
H	0.38821310840261	-0.19762121223218	3.91452179725348
H	0.73217169801259	-1.94308645895598	4.16646993288250
H	0.70303727304715	-0.87855490015501	-2.04779170409611
H	-0.66426182582538	-1.77671070156299	-1.35947777446751
H	-0.76530513778106	-0.00014806135777	-1.55917577602425

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Free carbene/BP86/6-311G(d)/Triplet state/300 degrees Constrained Optimization

C	0.08058678559636	-1.20460568509389	3.67085822594983
C	-1.37675068533289	-1.47321545227779	4.02070285515600
C	-0.08799766204184	-0.79978271548396	-1.28754526211263
C	0.49405609036157	-0.75597838447475	0.05171617072470
C	0.09505243628481	-0.43829833484232	1.40161772583878
O	-0.33304221664820	0.65961197848135	1.75527017402519
O	0.34890528625879	-1.47247129657794	2.26131036822121
H	-1.66556815858178	-2.49798743932890	3.74153897797107
H	-1.53237563849655	-1.35665118187092	5.10557753591808
H	-2.03864444131258	-0.76420426356772	3.50339044006328
H	0.35913583453343	-0.16332150830232	3.89061745393174
H	0.75964249916115	-1.88667199119997	4.20174310939192
H	0.69513705663134	-0.85921514528591	-2.06337339027345
H	-0.72964304778911	-1.69436389810153	-1.41510738082428
H	-0.70585703362448	0.09330210992656	-1.51304687198142

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Free carbene/BP86/6-311G(d)/Triplet state/310 degrees Constrained Optimization

C	0.07947315659380	-1.18414393686581	3.67941446614325
C	-1.37050004116374	-1.48003466462829	4.03742643913772
C	-0.07833587822017	-0.77643883942156	-1.29355359788021
C	0.49888935255531	-0.85643587590862	0.04779895247274
C	0.08073561252243	-0.50590309085392	1.38305894864467
O	-0.38175383088381	0.59278535135759	1.69098460851025
O	0.35867452141069	-1.49868113323560	2.28180898254715
H	-1.62995668756942	-2.52237029352060	3.79700478226783
H	-1.53156604789116	-1.32714413163661	5.11706871802578
H	-2.05090524464112	-0.80985469488612	3.49298884438930
H	0.32805829677699	-0.12758921914861	3.85899978304171
H	0.77634687792287	-1.82611891208199	4.23659755564569
H	0.69499632686199	-0.87895266359741	-2.07430224442328
H	-0.80620081924824	-1.59555687249779	-1.45855511523193
H	-0.60531849002641	0.18258576892532	-1.47147099129068

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Free carbene/BP86/6-311G(d)/Triplet state/320 degrees Constrained Optimization

C	0.08036965262441	-1.16897473900647	3.68385645068458
C	-1.36321126016904	-1.47936451333958	4.05580612092414
C	-0.07176432559541	-0.75622808969324	-1.29958280687824
C	0.47823953898358	-0.95854536433390	0.04155832300431
C	0.06313828521748	-0.57456894765479	1.36666707941285
O	-0.42418280739367	0.52575008733887	1.63315317782215
O	0.36340889565041	-1.52749797687174	2.29845298361739
H	-1.60291759303168	-2.53433102314052	3.85312527230746
H	-1.52489137210949	-1.29123200694506	5.12970763087617
H	-2.05733416013539	-0.84229972554988	3.48948089335507
H	0.30922410552673	-0.10234616198329	3.82630607225196
H	0.78983654760391	-1.77705137403179	4.26267223209798
H	0.70633394423284	-0.84784314730629	-2.07682369345922
H	-0.84094580450087	-1.51976370367336	-1.52866251888528
H	-0.54266654190381	0.24044347819103	-1.41044708513133

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Free carbene/BP86/6-311G(d)/Triplet state/330 degrees Constrained Optimization

C	0.07955620084177	-1.14063079022173	3.68708050630095
C	-1.34896550279998	-1.50366408840068	4.06977079974109
C	-0.05900448964953	-0.73317386017093	-1.30273563605105
C	0.45049356002852	-1.03455491271659	0.03696012660465
C	0.03650788754608	-0.62238357829118	1.35304414744564
O	-0.50086767988997	0.46350984642851	1.58151579113576
O	0.37896006331522	-1.52976945805222	2.31410593724147
H	-1.54083070496075	-2.57409505492991	3.90031063146139
H	-1.51972783106470	-1.28937349500569	5.13731066113688
H	-2.07093806809794	-0.91674411852935	3.48447859414988
H	0.26017664527539	-0.06096417019918	3.79656157481280

H	0.81510790305419	-1.69745615598675	4.28446070315444
H	0.68732371775079	-0.95732435151384	-2.08336670096627
H	-0.95308622559746	-1.34723708252894	-1.52896407750858
H	-0.35206837075163	0.33000806211846	-1.40526292665907

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Free carbene/BP86/6-311G(d)/Triplet state/340 degrees Constrained Optimization

C	0.07788204408582	-1.11544458136370	3.68775208805349
C	-1.33376234612145	-1.52462000701218	4.08640072519405
C	-0.04604736350399	-0.71377860580224	-1.30714253581916
C	0.40355934565062	-1.10468948326966	0.03119673903587
C	0.00411878826218	-0.66568382427718	1.34102707694171
O	-0.57549368109240	0.40513838143299	1.53987325627449
O	0.38830025974090	-1.53029915059959	2.32502611883776
H	-1.48286080561258	-2.60628414776996	3.94814439337330
H	-1.50976691969490	-1.28698087733598	5.14816598464609
H	-2.08063721748162	-0.98410668950691	3.48774949445926
H	0.21560911883359	-0.02682933787017	3.76680944907315
H	0.83707710645373	-1.62552118442584	4.29717653380074
H	0.66752658797447	-1.03059310415764	-2.08586792771618
H	-1.01879508306171	-1.18573178606902	-1.54940298436156
H	-0.18407272943266	0.38157119002707	-1.39163827979301

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Free carbene/BP86/6-311G(d)/Triplet state/350 degrees Constrained Optimization

C	0.07452103230620	-1.08958294649843	3.68627936676048
C	-1.31649605310885	-1.54847367686485	4.10289284962414
C	-0.03191753752047	-0.69723496093483	-1.31120418105886
C	0.34578502976814	-1.16521499060042	0.02493431070839
C	-0.03342204810014	-0.69978406607483	1.33056331242571
O	-0.65439857379395	0.35246247108107	1.50647292096674
O	0.39460063888226	-1.52246687134595	2.33154719374546
H	-1.42034956394859	-2.63845575021480	3.99130636850926
H	-1.49712967977047	-1.29300219556780	5.15974643236900
H	-2.08866564185317	-1.05450806923197	3.49611606291366
H	0.16687580746478	0.00536728224374	3.73933159653180
H	0.85787236594871	-1.55302772446207	4.30228924834113
H	0.63928073976590	-1.09830674679004	-2.08833348686919
H	-1.05989135274339	-1.01935281449513	-1.57052070588271
H	-0.01402805829694	0.40772785175628	-1.37615115708501

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Free carbene/BP86/6-311G(d)/RKS state/10 degrees Constrained Optimization

C	-0.41936320760001	-0.78856179844315	3.52687467970857
C	-1.87813278541785	-0.64597131584119	3.94175659659635
C	0.26609668678330	1.18389875942188	-0.81138478151110
C	-0.06120363564882	-0.04446053046397	-0.10108567567920
C	-0.23882186742478	0.26894078963688	1.38925427710796
O	-0.30066139342618	1.37278065508700	1.92050054983561
O	-0.29593914672209	-0.90142937450457	2.07722422186840
H	-2.48113064476572	-1.47746693088326	3.54743223408718
H	-1.95551584582507	-0.65555370694879	5.04086798358109
H	-2.29812428486218	0.30255714279432	3.57865136196846
H	0.17756786234219	0.07181687117798	3.86484873940070
H	0.02313139302076	-1.72109527970470	3.90315498544033
H	1.38650132758481	1.05755730723214	-0.79394806095615
H	0.02546170792908	1.15719075619093	-1.88565041377124
H	0.06448619603258	2.16014012824851	-0.32878372667697

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Free carbene/BP86/6-311G(d)/RKS state/20 degrees Constrained Optimization

C	-0.44298558177975	-0.68800606866524	3.55168288828133
C	-1.92898773836575	-0.69868014311949	3.88526746733936
C	0.74798473511924	1.04833269390350	-0.72821553820887
C	0.21174578146866	-0.10301949107515	-0.02238338520442
C	-0.22481508751945	0.24730699685298	1.36127779096020
O	-0.48983750073538	1.36711604587720	1.79325699683943
O	-0.22966067432162	-0.88445091907647	2.12222819307689

H	-2.40574200722487	-1.62233759852777	3.52453330012913
H	-2.06710645787958	-0.64344520157657	4.97733168466512
H	-2.43496714763647	0.16468339115034	3.43119401763088
H	0.02427846991954	0.26214086004953	3.85334183251709
H	0.08794311203140	-1.52913441547600	4.01867167373289
H	1.28114144910858	0.82380778175984	-1.66307749389724
H	-0.27976461594283	1.37172620649628	-1.06288736179189
H	1.16681689675829	1.91122968142702	-0.17250909506992

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Free carbene/BP86/6-311G(d)/RKS state/30 degrees Constrained Optimization

C	-0.43910504948304	-0.67591863005925	3.54952139615088
C	-1.92394861041475	-0.68952776828385	3.88631249348957
C	0.92396069358892	0.93041340686243	-0.71111453342711
C	0.21041321931804	-0.13378296211817	-0.02242450809941
C	-0.21801762056530	0.20983685722853	1.33972840365980
O	-0.50751650209590	1.34046058137265	1.73380998747290
O	-0.22652271207325	-0.90663815957909	2.12457678107983
H	-2.39444337930915	-1.62518465975578	3.54891962032831
H	-2.06091265934869	-0.60889939805566	4.97708279217467
H	-2.43653786602587	0.15844424786973	3.41128726513367
H	0.02194483371073	0.28435694507495	3.82805021262475
H	0.09979506929275	-1.50049848485389	4.03671239639858
H	1.42811349974303	0.62870224803588	-1.64065845758311
H	-0.01653850296070	1.44040954749138	-1.05576000146603
H	1.48746787562316	1.69283682777013	-0.13633087693729

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Free carbene/BP86/6-311G(d)/RKS state/40 degrees Constrained Optimization

C	-0.43619625251470	-0.67189147989002	3.57056072787408
C	-1.92795526752867	-0.67768181007035	3.87326274743325
C	1.05720155970266	0.79661472686184	-0.71442675543979
C	0.20714533863151	-0.15798033809716	-0.01537784100399
C	-0.16432891554836	0.15599897356438	1.34748943850164
O	-0.45880912476100	1.30452892085269	1.69814570101339
O	-0.18809916794599	-0.93788224336907	2.15660146261894
H	-2.39115151247453	-1.62073241472416	3.54639969471914
H	-2.09090215731620	-0.57196102837839	4.95839517811529
H	-2.42912272694644	0.15878466300813	3.36661142317141
H	0.02018161400526	0.29358990037394	3.83829824198555
H	0.09149373519953	-1.48396100380814	4.08997106775427
H	1.48713337366005	0.41721762447176	-1.65377002030714
H	0.23588597001242	1.47889339606132	-1.04953119781795
H	1.76988021582445	1.42468112214324	-0.14291689761809

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Free carbene/BP86/6-311G(d)/RKS state/50 degrees Constrained Optimization

C	-0.42996680825307	-0.73788119952685	3.61647488441523
C	-1.92998444798534	-0.64501950912035	3.85334380008381
C	1.05999450206280	0.74650843462044	-0.75166800438647
C	0.11863191813408	-0.06590663638182	0.01649582916450
C	-0.04830520286369	0.07185333394237	1.41387244538846
O	-0.22429634498530	1.25906814926064	1.76009088508328
O	-0.13160506474120	-1.01166328102356	2.21129615329546
H	-2.44064115197692	-1.55259526353234	3.49801529037097
H	-2.13439356704038	-0.53440230188389	4.93088912778069
H	-2.35267153399790	0.22604491149354	3.33312896748101
H	0.08190419992746	0.18937361105746	3.91642111048088
H	0.01917193588048	-1.58761256132962	4.14877373532509
H	1.65207644548166	0.04819134503816	-1.38279570013279
H	0.50277662840913	1.32965926437953	-1.50832313023716
H	1.75061843094817	1.40062534500630	-0.18630242311294

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Free carbene/BP86/6-311G(d)/RKS state/60 degrees Constrained Optimization

C	-0.42505914446944	-0.75844956316362	3.61408846968384
C	-1.92230824717719	-0.62758453721631	3.84792715804528
C	1.13492856305989	0.59094231064881	-0.75574766758858

C	0.06532024603510	-0.04980604521041	0.00826183701373
C	-0.02747101914155	0.04033426894664	1.41171380802691
O	-0.13794284906003	1.23708624896077	1.75866265949408
O	-0.13150271703841	-1.03876054619890	2.20712346685483
H	-2.45538967415413	-1.52203718279920	3.49235334896983
H	-2.12564380230719	-0.51097402031301	4.92499879215791
H	-2.32278268492802	0.25350100404134	3.32683649933847
H	0.11164164484173	0.15358179302038	3.91578158241029
H	0.00169336065759	-1.62031557103910	4.14503669844196
H	1.69716883888592	-0.24856802316943	-1.22721732195963
H	0.73990421548061	1.15253211879798	-1.61940960454292
H	1.85685337031511	1.20105832269406	-0.18069675534600

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Free carbene/BP86/6-311G(d)/RKS state/70 degrees Constrained Optimization

C	-0.42267615748617	-0.77231936101350	3.60774060723717
C	-1.91663870575164	-0.61845267899687	3.84634001100192
C	1.20082304159317	0.40780759989216	-0.75448250631330
C	0.02446699052324	-0.03370424010734	-0.00186842481910
C	-0.02039061859602	0.02207628467317	1.40449231914282
O	-0.07922758272694	1.22229660862744	1.75365152732975
O	-0.13953841441437	-1.05501755142118	2.19707211150691
H	-2.46494091953075	-1.50437955433003	3.49266102927730
H	-2.11451402283557	-0.49860173943396	4.92403132342146
H	-2.30587072792649	0.26874836344645	3.32692740954896
H	0.13078595250747	0.12963889150799	3.90804749497464
H	-0.00720194114214	-1.64209124978436	4.13451549260791
H	1.66400879341798	-0.54240391902505	-1.11221161882273
H	0.93976741356289	0.94982076664839	-1.67785059209755
H	1.97460340280533	0.95054246631668	-0.17935321299617

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Free carbene/BP86/6-311G(d)/RKS state/80 degrees Constrained Optimization

C	-0.42287368808001	-0.78261505398796	3.59938802940569
C	-1.91353142826290	-0.61655915965229	3.84681581601485
C	1.24408831299829	0.20782924960587	-0.75211227258414
C	-0.00270981926368	-0.00837712170695	-0.01010712630718
C	-0.01975815700733	0.02030582572344	1.39791704837800
O	-0.03651081723005	1.21946818798271	1.75497910614627
O	-0.15170491881317	-1.05915471215456	2.18321513112661
H	-2.47241765151306	-1.49529454269745	3.49162297847818
H	-2.10475185279320	-0.50077317841384	4.92620864366582
H	-2.29872472100894	0.27700144649210	3.33506866908411
H	0.14235639158412	0.11146498015073	3.90030029283880
H	-0.01169546192340	-1.66000822503693	4.11674511697274
H	1.56239707992748	-0.82982167525311	-1.01387989744702
H	1.09904997578169	0.71412746527234	-1.71940580692986
H	2.07995915660417	0.66234029367589	-0.18704275784286

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Free carbene/BP86/6-311G(d)/RKS state/90 degrees Constrained Optimization

C	-0.42363700587773	-0.78828396595601	3.58711097074464
C	-1.91283484156021	-0.62297756787979	3.84485469115224
C	1.25723581511730	-0.00311673237783	-0.74729628426165
C	-0.01530447848854	0.02559495501093	-0.01665392351279
C	-0.01843102163523	0.04302624094384	1.39408450229195
O	-0.00092562377326	1.23409077604110	1.77058575283876
O	-0.16265145090861	-1.04692152272826	2.16505965094321
H	-2.47492936779537	-1.49685193593890	3.48300900260044
H	-2.09766315995913	-0.51851966914556	4.92639714791432
H	-2.29953666501304	0.27667302227592	3.34496349186630
H	0.14502913407990	0.10063576813627	3.89546513548739
H	-0.01130013855441	-1.67283391901375	4.09112014958179
H	1.38614748613560	-1.10016556876553	-0.91695675516897
H	1.21156975838197	0.44676714482123	-1.75088013074486
H	2.15880955085076	0.33445737057636	-0.20115043073277

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Free carbene/BP86/6-311G(d)/RKS state/100 degrees Constrained Optimization

C	-0.42385513373123	-0.78838630364728	3.57574406017561
C	-1.91455475144993	-0.63642599511350	3.83362971131953
C	1.23303633506626	-0.22101445274864	-0.74047450851306
C	-0.01129516919395	0.05990517754939	-0.01686289539610
C	-0.00362300042769	0.08847226462501	1.39854697579635
O	0.04036006439076	1.26578624642321	1.80410207752170
O	-0.16025063926657	-1.01852741145657	2.14934991661775
H	-2.47112710355051	-1.50690302403194	3.45540524004735
H	-2.10229111612814	-0.55166259866399	4.91636133621984
H	-2.30601293316187	0.26951820978889	3.34881149065216
H	0.13947990495943	0.09768628462879	3.90064507163619
H	-0.00742927723242	-1.67973510629937	4.06433704935469
H	1.14546864501141	-1.33367255586412	-0.82268689337719
H	1.25770863461936	0.15249276305378	-1.77533155778443
H	2.19158803509510	-0.02679709424366	-0.22186410327040

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Free carbene/BP86/6-311G(d)/RKS state/110 degrees Constrained Optimization

C	-0.42204617367451	-0.78290780602872	3.56447125906903
C	-1.91815972326219	-0.65724999748392	3.80574164267082
C	1.16283058754850	-0.43931040783739	-0.72824943358539
C	0.00422287400268	0.09256666034107	-0.00941481481990
C	0.03626459739743	0.15300012540234	1.41229013158124
O	0.10869900136984	1.30977704584587	1.85653869102700
O	-0.13824053971484	-0.97670540516221	2.13758365896474
H	-2.45787269321669	-1.52712448803479	3.40235235810703
H	-2.12151401302797	-0.59702103725870	4.88730754328514
H	-2.31661298607843	0.25294488707230	3.33436120672293
H	0.12474371874748	0.10343929703871	3.91514036234895
H	0.00027245431611	-1.67891763275793	4.03974767365602
H	0.85369214905864	-1.51712627483887	-0.70952959269238
H	1.21919422077652	-0.16543638952615	-1.79249136329892
H	2.15865536975743	-0.40088343577161	-0.24613635203631

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Free carbene/BP86/6-311G(d)/RKS state/120 degrees Constrained Optimization

C	-0.41894641173490	-0.77150885345802	3.55385828077699
C	-1.92348166858538	-0.68459576265737	3.75840111287484
C	1.04225602143875	-0.64864235224988	-0.70768865272149
C	0.02578121994721	0.11836603583017	0.00643258660678
C	0.10675449493386	0.22027380249662	1.43299203203073
O	0.21563380905558	1.35157791340070	1.91840666153781
O	-0.09689849265223	-0.93247363483085	2.13269953950271
H	-2.43282955902169	-1.56023832203005	3.32864432215363
H	-2.15607199066200	-0.64492867812490	4.83503045517687
H	-2.33182261914545	0.22307830156274	3.29007509392506
H	0.09846467747948	0.12114702826290	3.93155292739640
H	0.01177147852465	-1.66548610052550	4.02609374198370
H	0.53469695329841	-1.64180909902264	-0.57251270431072
H	1.08427806767917	-0.48205185241614	-1.79438582505403
H	2.05228364244454	-0.76577194123778	-0.26988660087929

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Free carbene/BP86/6-311G(d)/RKS state/130 degrees Constrained Optimization

C	-0.59384506296070	-0.43415142700499	3.47656171280264
C	-1.98197346557545	-0.98834839793281	3.73728277374853
C	0.79717355496055	-0.86505118569652	-0.70141901536660
C	0.55922910222540	0.33947270498060	0.08531922887617
C	0.61187115923739	0.25370615942080	1.52267036248233
O	1.28774651748898	1.05029763197113	2.17524502717159
O	-0.29241000659645	-0.62627276104235	2.05936448873491
H	-2.04188006600438	-2.05395801598785	3.46862506340650
H	-2.23111057294142	-0.89123000989070	4.80597558032662
H	-2.74104131812830	-0.44201837241781	3.15761021483224
H	-0.51169338121119	0.63880090624082	3.71025700976819
H	0.17868795130165	-0.96135386028576	4.05913601271634
H	-0.26064747347942	-1.23425147592178	-0.60822771378168

H 0.96170639633605 -0.70469547943921 -1.77716972755551
H 1.43326469834731 -1.67821432499358 -0.30151804716227

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Free carbene/BP86/6-311G(d)/RKS state/140 degrees Constrained Optimization

C -0.59584193899613 -0.43595271916583 3.46230454333781
C -1.98148012322310 -1.00224897888649 3.71014219772362
C 0.62272999267411 -0.99265585335101 -0.67388399066469
C 0.58168498853052 0.25565050248409 0.07564007397788
C 0.66353688311202 0.20701609410036 1.52250365734270
O 1.31120765663090 1.01491393961110 2.18390160268178
O -0.25858354805838 -0.66642610775186 2.06083755411340
H -2.02084363504368 -2.07630690124108 3.47309110691585
H -2.25544931455450 -0.87674793394594 4.76975161521216
H -2.73567286222272 -0.48473162782702 3.09838538180687
H -0.53203087770559 0.64493606334949 3.66467923012913
H 0.17123861573408 -0.93210066033418 4.07873782664593
H -0.47230063093546 -1.19824064398258 -0.52174054376822
H 0.75144022141662 -0.88756052068311 -1.76131300690408
H 1.15346723864133 -1.87776581737593 -0.27332427755015

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Free carbene/BP86/6-311G(d)/RKS state/150 degrees Constrained Optimization

C -0.42101109574124 -0.74810401787270 3.52198646700134
C -1.93716504363373 -0.73544119547548 3.65069479449997
C 0.53684557367150 -1.11767810914138 -0.62656306300200
C 0.05447795266493 0.09664047280797 0.01249286522732
C 0.26479317068924 0.28235823878132 1.44447540428216
O 0.40396576765338 1.36871478412526 1.99459557654351
O -0.02593102557170 -0.89630036005921 2.12280559942711
H -2.38177267078520 -1.64150418951424 3.21165924556736
H -2.22627039385634 -0.69213567820500 4.71329960495005
H -2.36680180916497 0.14392056187547 3.14790952158854
H 0.03409052010505 0.17134843178375 3.91537541973691
H 0.02735606135753 -1.61739279778565 4.02500790666233
H -0.35961714490624 -1.71358486783538 -0.30208456262540
H 0.49662937106744 -1.11618254424298 -1.72599162992680
H 1.41981036845036 -1.65898005624175 -0.23595017893241

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Free carbene/BP86/6-311G(d)/RKS state/160 degrees Constrained Optimization

C -0.41181456256357 -0.80682948816694 3.50283545536888
C -1.91739171553594 -0.67030808939697 3.68354761945279
C 0.40731697159120 -1.20790801213043 -0.61202236666741
C -0.02156720046789 0.06308652402418 -0.05135997480866
C 0.13062861737284 0.26135373368995 1.40507008959144
O 0.14983618872509 1.35570744929247 1.95499546243505
O -0.06093969371602 -0.92963249703338 2.08927679219147
H -2.45084301045821 -1.51599944133672 3.22345832377431
H -2.16765460358060 -0.65074981197514 4.75658036652810
H -2.28389664910369 0.26425538727418 3.23443924210922
H 0.12695042079435 0.05457792645082 3.92089885065377
H -0.02718237661784 -1.73332319024783 3.95255562666797
H -0.56763422050677 -1.70324169284461 -0.34320616219563
H 0.44391893054331 -1.24428180530723 -1.71115496852129
H 1.20109261452375 -1.81507472229235 -0.13620138558002

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Free carbene/BP86/6-311G(d)/RKS state/170 degrees Constrained Optimization

C -0.41802191358338 -0.82831645590225 3.48771209432328
C -1.91060611881678 -0.64519337985452 3.72672074242193
C 0.24931420773353 -1.27171769739119 -0.60577508590724
C -0.01519201687769 0.07080559640606 -0.11491455114128
C 0.04566898793265 0.24450093151057 1.37504528568728
O 0.02251076893858 1.33881584336847 1.92195974694248
O -0.12037120933376 -0.94134534350722 2.06093133125863
H -2.48782294674980 -1.46598881595520 3.27440596866085
H -2.11933273882061 -0.63646372656363 4.80870113377165

H	-2.26204876293073	0.30843176305796	3.30738725793474
H	0.16202314932132	0.01075147412149	3.89676655549079
H	-0.04852589558661	-1.77323729084873	3.91054161414794
H	-0.82738950670824	-1.57475765741951	-0.45366418097763
H	0.39989350856068	-1.34647514697889	-1.69344516605116
H	0.85669329092082	-1.99789372004341	-0.03265977656228

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Free carbene/BP86/6-311G(d)/RKS state/180 degrees Constrained Optimization

C	-0.42707074480838	-0.83485383947924	3.48299962861533
C	-1.90228279864724	-0.62976092687018	3.79862461532915
C	0.07803741985830	-1.30624808590886	-0.62025521295506
C	0.05028858868382	0.07640111029404	-0.16789773617869
C	-0.06787972665103	0.22280330058346	1.34636055479542
O	-0.10372562810486	1.32050844314748	1.88130451351385
O	-0.20372105620568	-0.95185141085295	2.04288563579450
H	-2.51388025371718	-1.44020461165310	3.37373884958068
H	-2.05404848791823	-0.62349563486265	4.89002483173030
H	-2.25929087809412	0.33114596508754	3.40177656710305
H	0.18354124639905	-0.00151607488269	3.85957611872466
H	-0.04933755271757	-1.78371007219388	3.88907821319372
H	-1.04850426402771	-1.36001332094180	-0.70419601552516
H	0.42526224051162	-1.44111856612990	-1.65621782099990
H	0.37104531543922	-2.13457549233725	0.05191022727813

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Free carbene/BP86/6-311G(d)/RKS state/230 degrees Constrained Optimization

C	-0.38684351273046	-0.73677539634668	3.54087335072501
C	-1.83849188019022	-0.77276768917686	3.99684854924002
C	0.01086453628467	-1.24729483534622	-0.77111400197581
C	0.54731849789470	-0.23051304813605	0.13231699547291
C	-0.21522284595076	0.13706516915722	1.29914322204002
O	-0.50551829528574	1.27048697695408	1.66451118533796
O	-0.29433814428849	-0.99156527046205	2.10463052526329
H	-2.31475786597601	-1.72722229061526	3.72563297599236
H	-1.88965545231134	-0.66379235476817	5.09274819939662
H	-2.40648442144970	0.05026761155896	3.54100093130504
H	0.06944222326796	0.24274605820630	3.75059166518190
H	0.21264125141608	-1.53356921892624	4.00416292509903
H	-0.58008483500121	-0.64047972770345	-1.50295984636407
H	0.78139240833768	-1.75026284712874	-1.37550809246896
H	-0.71182824401715	-1.96281235426683	-0.33316561424531

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Free carbene/BP86/6-311G(d)/RKS state/240 degrees Constrained Optimization

C	-0.37182870527386	-0.70929960818833	3.60884641017238
C	-1.85140936930300	-0.79386801457369	3.95298226504781
C	-0.02890270529109	-1.19714652234286	-0.81614542059977
C	0.60069672855242	-0.26687275053591	0.12496089844801
C	-0.09849522601065	0.03392166939546	1.34301028719873
O	-0.43662570143477	1.18567534385101	1.62325685632839
O	-0.14680050183212	-1.03471462962957	2.19977864819122
H	-2.26077579156215	-1.78311899623145	3.69753761113970
H	-1.99593979566139	-0.63249369239334	5.03385305789573
H	-2.41921055888045	-0.02390804487026	3.41169849073033
H	0.02463214363941	0.29924079282769	3.80060288747363
H	0.22420064606016	-1.45111802185584	4.15902928558145
H	-0.80631862976686	-0.59112475472345	-1.34176061684042
H	0.64756373011958	-1.57737975520374	-1.59565830181831
H	-0.60235284335521	-2.01428223252571	-0.33227938894888

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Free carbene/BP86/6-311G(d)/RKS state/250 degrees Constrained Optimization

C	-0.39894478339831	-0.71003348449867	3.67854915877263
C	-1.90361915557565	-0.69403951368401	3.89801056588776
C	-0.12461211768194	-1.10582751345942	-0.88276956557753
C	0.65147870222329	-0.40562996181043	0.14155827160380
C	0.05553173110669	-0.13993042026639	1.40559342728631

O	-0.18507692752524	1.06292592126121	1.59732857022797
O	-0.07059308608832	-1.13501990591391	2.31395637443054
H	-2.34767223404017	-1.67287263799939	3.66097144387510
H	-2.12845661957072	-0.46298134322198	4.95202994898093
H	-2.38054838563116	0.07281090549724	3.27097988304971
H	0.04401207562421	0.28196736900442	3.85079786941013
H	0.10427464397419	-1.45049253409341	4.31570508496367
H	-1.22995748354738	-1.05424591318630	-0.84595715369693
H	0.24907480223146	-0.99270209440104	-1.91150364589162
H	0.14354225789903	-2.15041809022793	-0.57553726332249

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Free carbene/BP86/6-311G(d)/RKS state/260 degrees Constrained Optimization

C	-0.39492929355976	-0.67385292012054	3.72250416162617
C	-1.90413975721669	-0.70411915254367	3.90538525032686
C	-0.12706917826931	-1.08017826651685	-0.90978410098604
C	0.68109258924157	-0.50965918788195	0.17283465760225
C	0.08345907748133	-0.24641240858081	1.42806376347487
O	-0.19616450555508	0.96422363244014	1.52636857726354
O	-0.01352955345711	-1.17589001655862	2.39731587687923
H	-2.30354173366611	-1.71341152325192	3.72313504629697
H	-2.16440512965768	-0.41466258523432	4.93653138923432
H	-2.39538356399068	0.00053257288121	3.21908626350972
H	0.00697647342167	0.34310198751564	3.83962663107998
H	0.11931406703546	-1.35087484337269	4.41845255931533
H	-1.22396328067629	-0.93617989239716	-0.86993879179062
H	0.26188523936265	-0.89048186243306	-1.92168796513669
H	0.04883196950600	-2.16862475094541	-0.71818034869591

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Free carbene/BP86/6-311G(d)/RKS state/270 degrees Constrained Optimization

C	-0.36637858671776	-0.64966915761766	3.75079838754895
C	-1.87420349113353	-0.70194820010912	3.93933604317134
C	-0.17081450743915	-1.05477021825036	-0.94331300771519
C	0.67492380488576	-0.63997605103523	0.18204926702877
C	0.09522059807727	-0.35162408519114	1.43506163006047
O	-0.19431835905765	0.86359325388501	1.45972974600332
O	0.02343351055225	-1.22047193125971	2.45579060680744
H	-2.25181568255615	-1.72839896042704	3.81643156879530
H	-2.13916546161228	-0.35923665451073	4.95276950131940
H	-2.38280996298990	-0.04887228236452	3.21549051614410
H	0.01520310039824	0.37990888193874	3.80815620476826
H	0.16314773388056	-1.27483757327204	4.48273451569882
H	-1.24617833318732	-0.79956331478818	-0.88339573976622
H	0.24059785374495	-0.80256928490963	-1.93268782978810
H	-0.10840879684529	-2.16805363908842	-0.86923844007670

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Free carbene/BP86/6-311G(d)/RKS state/280 degrees Constrained Optimization

C	-0.35090045780703	-0.61523349972252	3.77067976364055
C	-1.85760850429337	-0.73854470683558	3.93684012813498
C	-0.14823517243109	-1.04675218308028	-0.95786948730160
C	0.68375880914399	-0.70859505666138	0.20426154092686
C	0.08511226966797	-0.39896769649257	1.44158588570426
O	-0.30752497096119	0.78801875143374	1.40453913827408
O	0.09736552126968	-1.21374006830487	2.50836089342209
H	-2.17917250486866	-1.78746257787678	3.84854743151302
H	-2.15734995876062	-0.37272055308379	4.93237824983328
H	-2.38701150411436	-0.14092575815946	3.18096022218094
H	-0.02247796338483	0.43376866445067	3.79680752964907
H	0.19450040108633	-1.18479475990959	4.53547149315394
H	-1.12256100732294	-0.51940005952596	-0.95741989467235
H	0.35476513974673	-0.92468035142346	-1.92809903211329
H	-0.40422667697062	-2.12645936180818	-0.84733089234585

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Free carbene/BP86/6-311G(d)/RKS state/290 degrees Constrained Optimization

C	-0.34895535202540	-0.54357813109971	3.78224867356846
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C	-1.81718336087273	-0.87131855389434	4.00651624325228
C	-0.14592377680650	-1.07715665833478	-0.98384360911539
C	0.63864362937216	-0.76198604555386	0.21463519915601
C	0.02251378788246	-0.39135767556114	1.43316776472853
O	-0.49673022112931	0.74040717974892	1.35813322743269
O	0.14475482082067	-1.14666618724026	2.54078346481026
H	-1.98561845878213	-1.95876849973062	3.98665609484383
H	-2.14173337100664	-0.49278398182721	4.98942560117643
H	-2.44627045040707	-0.40216519744932	3.23623779768867
H	-0.17663604498907	0.54119154703404	3.73828067527218
H	0.29327208989963	-0.98180007250577	4.55850675815194
H	-0.42307714873750	-0.06463642100264	-1.34966112474455
H	0.45863060885467	-1.51588112330948	-1.79228419089299
H	-1.09725333207325	-1.62998939627387	-0.84908960532835

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Free carbene/BP86/6-311G(d)/RKS state/300 degrees Constrained Optimization

C	-0.35768019276525	-0.49110868304430	3.79600569316545
C	-1.76668521186317	-1.00544098397425	4.04980780242210
C	-0.15550823732346	-0.91054132161613	-1.02841465519460
C	0.58454741663208	-0.68171864112918	0.21187755246092
C	-0.03755846332719	-0.38367584916757	1.43942368047504
O	-0.69728318763945	0.67383962673908	1.32565863056297
O	0.20380209303014	-1.06669033632970	2.57140102534120
H	-1.78620748311085	-2.10565512662405	4.07012989602370
H	-2.13267733744355	-0.63856391848416	5.02247001472266
H	-2.46048537078111	-0.65481313509920	3.27186653369297
H	-0.33205218003826	0.60466762037238	3.71402568363038
H	0.34286178779379	-0.81104743387128	4.57957546914524
H	0.25791873487791	-0.31873162472320	-1.86275622939372
H	0.07103662345970	-1.96260222562540	-1.31847697591027
H	-1.25559557150132	-0.80440718442306	-0.97288115114403

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Free carbene/BP86/6-311G(d)/RKS state/310 degrees Constrained Optimization

C	-0.36001110087321	-0.47557160367899	3.80676348718054
C	-1.76766095615117	-0.99492151667888	4.06144209625195
C	-0.15711772902373	-0.92434810387165	-1.03723017183095
C	0.55885742516286	-0.81959103242634	0.23183300003626
C	-0.04715277318031	-0.43065195328655	1.44562199276359
O	-0.70940641883366	0.62119554118210	1.31089864651562
O	0.21603229287266	-1.07144167609869	2.60088912629088
H	-1.77882175948833	-2.09449727440736	4.10662434158637
H	-2.14379284991476	-0.60884632014800	5.02271269569641
H	-2.45847982631503	-0.66761999179250	3.27082105890225
H	-0.34200144164545	0.61847469249353	3.70368468302214
H	0.33587574932932	-0.77386803339845	4.60289069323449
H	0.26994835243980	-0.19700401118297	-1.75246237367116
H	0.12259943857777	-1.89804646681413	-1.49473620634325
H	-1.26043498295675	-0.83975146689113	-1.01004009963515

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Free carbene/BP86/6-311G(d)/RKS state/320 degrees Constrained Optimization

C	-0.35498748765997	-0.44708992908051	3.78441884122417
C	-1.76521631680531	-0.98892883995799	3.97418935529441
C	-0.21657518034625	-1.06384807252695	-0.94873429779946
C	0.57735813300312	-1.06303000488094	0.27229153818438
C	0.01837302742995	-0.37299763986804	1.42062880437897
O	-0.58090986798050	0.70159212045604	1.30946047831362
O	0.27598164173428	-1.01228521067711	2.59408027997741
H	-1.76375615205668	-2.08916645421407	4.00157318927072
H	-2.18473937811593	-0.62295463012312	4.92520427325271
H	-2.42860548832641	-0.65663190447573	3.16224495085451
H	-0.34838135248470	0.64822971488983	3.69712699242867
H	0.31242411532579	-0.75084069359218	4.60261277158653
H	0.12243430382468	-0.06047301438610	-1.31177804917204
H	0.13782274282851	-1.76209625965521	-1.72184706614867
H	-1.32278932037057	-1.01596839890795	-0.89175909164592

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Free carbene/BP86/6-311G(d)/RKS state/330 degrees Constrained Optimization

C	-0.36117673345033	-0.41963330275913	3.77427048188192
C	-1.74854040983938	-1.01438783210417	3.97635259010990
C	-0.22441918741101	-1.06334212304738	-0.93942833484992
C	0.54725527424494	-1.16216484148109	0.28849965158771
C	-0.00530835267421	-0.37166734060654	1.40413607011006
O	-0.64373782389572	0.67420461090794	1.28961005784180
O	0.28748076402280	-0.97790360907248	2.59094456347107
H	-1.70287089410611	-2.11297987406969	4.02186272374658
H	-2.17996914402505	-0.64946776467415	4.92229592934918
H	-2.42630811666114	-0.72186608910109	3.16108766413484
H	-0.39947628160190	0.67334240065683	3.66722515756065
H	0.31961655082596	-0.68429059555087	4.59495027960037
H	0.27883598179041	-0.10602052025065	-1.24975243232250
H	0.04614443742944	-1.78439465304760	-1.72407922990329
H	-1.30909264464868	-0.83591768279993	-0.90826220231837

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Free carbene/BP86/6-311G(d)/RKS state/340 degrees Constrained Optimization

C	-0.36687497329878	-0.39968486305579	3.76690717842251
C	-1.73358678002202	-1.02376810224548	4.01724244941037
C	-0.20487745588012	-1.04002792600576	-0.96544542880444
C	0.50502614565205	-1.24688790689792	0.28440737603852
C	-0.07342846302191	-0.41431443621203	1.38843068103227
O	-0.77262871381005	0.58827955285770	1.26848339111227
O	0.26789933013582	-0.97361643597183	2.58383525826626
H	-1.65784914641923	-2.11903986808626	4.09166288681860
H	-2.15178778178408	-0.64349242381225	4.96299538948679
H	-2.43693201572969	-0.77094581334451	3.21067671051466
H	-0.43775167875752	0.68859662158653	3.63027018556236
H	0.33906404653743	-0.62495294264154	4.57796713836223
H	0.43332581737997	-0.14045115929312	-1.20876307867303
H	0.02030740310819	-1.76086916036374	-1.76418293314522
H	-1.25147231409006	-0.67531435351401	-0.97477423440414

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Free carbene/BP86/6-311G(d)/RKS state/350 degrees Constrained Optimization

C	-0.37577200831003	-0.38471301374012	3.75592397286497
C	-1.71912774526952	-1.02547192399816	4.08015322989568
C	-0.16376370675883	-0.99776511847130	-1.00715825297689
C	0.44963263520633	-1.32964899348465	0.26612682203112
C	-0.17079452574594	-0.48729531208247	1.37225665028451
O	-0.92902529389587	0.46894221382503	1.24861827080255
O	0.22587703013274	-0.99107824553750	2.57177328833256
H	-1.61749068596962	-2.11531808303330	4.19248872873846
H	-2.10910569277403	-0.61756386519599	5.02643396625219
H	-2.45639887519733	-0.81668687887395	3.29178999563163
H	-0.47633491821769	0.69605146042398	3.58087644526467
H	0.36412368441970	-0.56562443182595	4.54752270378832
H	0.58650517910695	-0.16781188620833	-1.17876715966008
H	0.03018659046621	-1.70706666989155	-1.82454030273374
H	-1.16007824719307	-0.51543846890575	-1.05378538851595

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Free carbene/BP86/6-311G(d)/BSS state/0 degrees Constrained Optimization

C	0.00847713158337	-1.36995275782899	3.39183997694653
C	-1.41168599852203	-1.30508533288546	3.93885993006879
C	-0.00235075939183	0.98584357127076	-1.03630270701685
C	0.01064306234063	-0.08313414596615	-0.04193213284317
C	-0.01026465146066	-0.07114328526780	1.38624029706480
O	-0.04658197860975	0.98020885049406	2.04002960834166
O	0.02187292661951	-1.32119986319234	1.93590490021184
H	-2.03676982996142	-2.09865619127960	3.50206535699047
H	-1.40092710653996	-1.43916417457497	5.03282820248845
H	-1.87076805001600	-0.33075155033802	3.71922020760329
H	0.62425435886667	-0.54541543472074	3.78109019640880

H	0.49181449256705	-2.32854786882938	3.62722774972677
H	-0.90117667522269	0.93184327965611	-1.68034860444333
H	0.01467239725837	1.98184567793862	-0.55331988389504
H	0.86648145548872	0.91836317152392	-1.71813296465302

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Free carbene/BP86/6-311G(d)/BSS state/10 degrees Constrained Optimization

C	-0.00858906060321	-1.43708157428839	3.33765850163566
C	-1.36996457653441	-1.21817316728800	3.98465829152316
C	0.12266244584374	0.97591107703430	-1.01692428326673
C	-0.11043591181183	-0.14145195300902	-0.10046256437481
C	-0.02085859570948	-0.12757957248774	1.33874758882329
O	0.10008056025156	0.91409588448578	1.99279951803736
O	-0.09502041251914	-1.37520243841631	1.88407646135912
H	-2.10991860336247	-1.93238186560521	3.59293132000643
H	-1.29589741958014	-1.36314551462886	5.07475143631282
H	-1.73059422849200	-0.19637100231949	3.80006571202089
H	0.72196727590811	-0.68995808727780	3.68236380387950
H	0.37915334142284	-2.44613576823142	3.53558371928000
H	-0.32376245194668	0.80451796466869	-2.00967695221035
H	-0.28327680920789	1.91834678518881	-0.59926798644164
H	1.20865323534101	1.14778584517465	-1.17203443358470

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Free carbene/BP86/6-311G(d)/BSS state/20 degrees Constrained Optimization

C	-0.00316736785060	-1.42146773471762	3.34436844589845
C	-1.37773327683765	-1.24126500005337	3.97491480532390
C	0.29580969899857	0.93697970566619	-1.01403269678141
C	-0.09779996942000	-0.13137092825853	-0.09500017235224
C	-0.02351935290249	-0.11468458829081	1.34410183418092
O	0.05041702617097	0.93107666861449	1.99868950088890
O	-0.07574867581211	-1.36376666881781	1.88963448934177
H	-2.09206904601081	-1.97697874390594	3.57555210541300
H	-1.31248861770664	-1.38246285540794	5.06611985687910
H	-1.76496204757602	-0.23053721714195	3.78377356110484
H	0.70095831067947	-0.65255763055522	3.69642295996790
H	0.41181293493340	-2.41845616362760	3.54820285085473
H	-0.30613488807242	0.94253146104030	-1.93777205532038
H	0.22588586329939	1.92699400359612	-0.52302257832215
H	1.35440832910694	0.81483533785972	-1.32668277407734

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Free carbene/BP86/6-311G(d)/BSS state/30 degrees Constrained Optimization

C	-0.00371351491748	-1.42116459445934	3.33998788927761
C	-1.37620933938203	-1.24469293321486	3.97539588501311
C	0.45316805030360	0.87289889127582	-1.00586014984998
C	-0.11305603377421	-0.12774140681753	-0.10047372681311
C	-0.02850772730661	-0.11874988986493	1.33749098929002
O	0.03855104801675	0.93030822566608	1.98764265460281
O	-0.08315214081384	-1.36603135035397	1.88472216759893
H	-2.08954860642113	-1.98341024645368	3.57987060953091
H	-1.30640616271835	-1.38382373291761	5.06662174247568
H	-1.76726617136852	-0.23560146148451	3.78370227850488
H	0.69930885586924	-0.64930630352023	3.68798013684497
H	0.41591258108964	-2.41631937600364	3.54324069454932
H	-0.15296261096823	1.01492611947782	-1.91574210154187
H	0.59050504039931	1.84427677620655	-0.49259123355973
H	1.46112563799186	0.55307593946403	-1.34671770292355

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Free carbene/BP86/6-311G(d)/BSS state/40 degrees Constrained Optimization

C	-0.00619387636827	-1.42610359922623	3.33360371270624
C	-1.37392163433720	-1.24336487163760	3.97660947214179
C	0.59317302291540	0.78477555313265	-0.99700984062531
C	-0.13692194205377	-0.11797503803124	-0.10529946556070
C	-0.03045845694813	-0.12696317945909	1.32960987205973
O	0.04510289579799	0.92539849654170	1.97399780285465
O	-0.09466014591288	-1.37172300607408	1.87773099141833

H	-2.09270900270594	-1.97927515745294	3.58579590310222
H	-1.29842603541761	-1.38194754931622	5.06755384060916
H	-1.76165867116647	-0.23278762848720	3.78610500929278
H	0.70262049947257	-0.65738525209561	3.67672182061382
H	0.41080540523731	-2.42283295897469	3.53442736534340
H	0.03046525141257	1.03482348607296	-1.91094597031454
H	0.89582511910404	1.71198471615749	-0.47275955971999
H	1.53454474497037	0.29651904185010	-1.33087082092156

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Free carbene/BP86/6-311G(d)/BSS state/50 degrees Constrained Optimization

C	-0.00728089810221	-1.42595452723177	3.33873258351559
C	-1.37998627261450	-1.24553417829614	3.97106968268760
C	0.71411816774343	0.67796132058257	-0.98859532196358
C	-0.15154165951304	-0.10183889831385	-0.10169306714524
C	-0.01681328561099	-0.14301988264912	1.32610585572799
O	0.06786685719924	0.91848418168616	1.95731125448939
O	-0.08792469176032	-1.38050879705257	1.88108490869895
H	-2.09315437481027	-1.98667918254858	3.57994466489274
H	-1.31125532325855	-1.37704826229846	5.06335030730328
H	-1.77099962304781	-0.23788641705113	3.77154985093774
H	0.69592322732404	-0.65229162800074	3.68183609592311
H	0.41354704870259	-2.41922955953600	3.54816546510441
H	0.19041364586028	1.05588478315095	-1.88150441136515
H	1.21676777435277	1.50953459003001	-0.45796923676325
H	1.52484659153534	0.01493916852868	-1.36411850004361

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Free carbene/BP86/6-311G(d)/BSS state/60 degrees Constrained Optimization

C	-0.01013992011272	-1.43337117028182	3.34239647344818
C	-1.38548420707737	-1.24142104699892	3.96439221041583
C	0.81047903396091	0.55367164310638	-0.98055634561715
C	-0.17064917292286	-0.07469573823433	-0.09248175565564
C	0.00034556661121	-0.16160029427088	1.32434239234607
O	0.10893960140711	0.90702085997381	1.94375918875483
O	-0.08137189132618	-1.39287053137658	1.88228126024172
H	-2.10112480639998	-1.97917891424016	3.57148429949051
H	-1.32511208366799	-1.36874330264396	5.05766578506193
H	-1.76875678925344	-0.23204594768395	3.75836800921462
H	0.69710605120368	-0.66413140361639	3.68660625161535
H	0.40303941928932	-2.42863555974791	3.55693414487345
H	0.35731867062090	1.02448899708564	-1.86747051810365
H	1.47081847275155	1.27115789069908	-0.45635328907752
H	1.47532711891585	-0.25217650177004	-1.36609797500853

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Free carbene/BP86/6-311G(d)/BSS state/70 degrees Constrained Optimization

C	-0.00942641013254	-1.43219535271472	3.35705623889821
C	-1.39648892150940	-1.24208562499458	3.95170010762270
C	0.88435526503931	0.41599919727502	-0.97328940251939
C	-0.17828940865381	-0.04737039191855	-0.07616718223990
C	0.02445379443891	-0.18793202735750	1.32483791526722
O	0.14697869622263	0.89431764179264	1.92431923129783
O	-0.05540767108520	-1.40936858262302	1.89327018108771
H	-2.10018347906422	-1.98964368109686	3.55586054572511
H	-1.35470651169418	-1.35486342772750	5.04741042507241
H	-1.78345045977437	-0.23817769495829	3.72635687127655
H	0.68824979589929	-0.65557685455453	3.70347488172560
H	0.40669844606708	-2.42218132885108	3.58888474182663
H	0.51020696222995	0.97943840920041	-1.84261752275034
H	1.69660746759269	0.97192838317260	-0.46694093382989
H	1.35214390742385	-0.50653528764403	-1.38888596646043

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Free carbene/BP86/6-311G(d)/BSS state/80 degrees Constrained Optimization

C	-0.00460870073112	-1.42364940904766	3.38483298963844
C	-1.41088742602553	-1.24728955348394	3.93526855475616
C	0.93308500318507	0.27801483832763	-0.96230479026903

C	-0.17645258966830	-0.01765087060185	-0.04978835000255
C	0.05796389301015	-0.24426525714653	1.32100978540313
O	0.19359300680373	0.86704697970410	1.87845481272778
O	-0.01247630006499	-1.44429830020129	1.91720765572437
H	-2.08681688008972	-2.02287642640699	3.54520075267504
H	-1.39629937548978	-1.32455798989358	5.03468471216349
H	-1.81480077121269	-0.26027155363228	3.66828309065367
H	0.66871063429044	-0.62346391123096	3.72492518646676
H	0.42697123466190	-2.39695561982084	3.65485416450081
H	0.65839674094395	0.95396324151806	-1.78716111774508
H	1.88544829398945	0.59019436213177	-0.49314911102458
H	1.12505449839745	-0.70943412921566	-1.44704820366841

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Free carbene/BP86/6-311G(d)/BSS state/90 degrees Constrained Optimization

C	-0.00072442087792	-1.43245338295031	3.37845747648020
C	-1.41342584968795	-1.29283803782134	3.92268675247923
C	0.94898765347519	0.13943180422245	-0.96504747388947
C	-0.17461431352524	0.05109043299445	-0.02512474171579
C	0.06604485258683	-0.20281505560527	1.34156649842043
O	0.21085462401410	0.89305241489183	1.92357357900151
O	-0.00044511687338	-1.41759006399082	1.9099579877151
H	-2.07349985035435	-2.07072104779095	3.51067481552544
H	-1.40516324015546	-1.39410876148428	5.02019780681447
H	-1.83313670484432	-0.30721223169959	3.67518460222786
H	0.65746435302051	-0.62998184925108	3.74112631237713
H	0.44556094608129	-2.40463596731502	3.62789089111451
H	0.75405577661536	0.77435851133603	-1.84287514316866
H	1.94786240449217	0.34906098186017	-0.53669617580250
H	0.98979640303317	-0.90656421339627	-1.35634086663589

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Free carbene/BP86/6-311G(d)/BSS state/100 degrees Constrained Optimization

C	0.08040487133777	-1.17166966435594	3.46325991623992
C	-1.34910215714502	-1.40940187086950	3.92320180758151
C	0.91412339927857	-0.14189239268396	-1.00333735568496
C	-0.24348201791292	-0.19383311646257	-0.10484509217713
C	-0.04183717326905	-0.18340915393157	1.29637004758347
O	-0.23342226663711	0.96053434075276	1.75153004976759
O	0.18967140418769	-1.30521233744368	2.00492744994391
H	-1.71697968314062	-2.38755544557732	3.57894703147586
H	-1.39798130819141	-1.39122648704852	5.02415762145208
H	-2.01984859195770	-0.62667632294551	3.54036096541973
H	0.44354929438796	-0.17615787279485	3.75514505754938
H	0.77162369467154	-1.93434728405682	3.84701708625266
H	1.85822953167918	0.28273745922012	-0.61101675951295
H	1.09658903428326	-1.23904627112896	-1.12769398179603
H	0.69620215142785	0.23872193932633	-2.01275371209502

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Free carbene/BP86/6-311G(d)/BSS state/110 degrees Constrained Optimization

C	0.08633150396172	-1.19933357250775	3.42889777469122
C	-1.34151434037446	-1.41586590039795	3.90575758815211
C	0.84729367581721	-0.34751848861490	-1.00724528171401
C	-0.26724665180451	-0.11267297295614	-0.08395517999307
C	-0.04606614550142	-0.05362864809310	1.32883189676436
O	-0.16756433586796	1.05041562494447	1.87185606853552
O	0.16117333676671	-1.23728869352918	1.96519919381478
H	-1.75315386429830	-2.35461444043665	3.50558142067524
H	-1.36783753476562	-1.46982095042893	5.00631187609077
H	-1.99046262700930	-0.58549895225300	3.59158795559786
H	0.4918968819322	-0.23919004731498	3.77728860373021
H	0.75542093424225	-2.01098202254780	3.74659873200907
H	1.83053665849927	0.06954720267552	-0.71301477398284
H	0.96782166319024	-1.45565383116236	-0.93801687056317
H	0.62680425595095	-0.11779891837724	-2.06040887180806

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Free carbene/BP86/6-311G(d)/BSS state/120 degrees Constrained Optimization

C	0.08806646690591	-1.23063602105508	3.40476496569813
C	-1.34474984354755	-1.41638993050491	3.88110006100644
C	0.74414458734585	-0.52766224737167	-1.00081123006780
C	-0.26825439400590	-0.04279139805832	-0.05753919511143
C	-0.01507427243578	0.02409131684555	1.35810547829733
O	-0.07293908048965	1.09686612087374	1.95978059994970
O	0.15463681182091	-1.20293589193168	1.94220768646647
H	-1.79306465510469	-2.32024545634628	3.44177825282724
H	-1.36753111170626	-1.51924712174381	4.97823436258952
H	-1.96425901904020	-0.54924987852209	3.60950555661279
H	0.52971951321751	-0.30240542610779	3.79319635598878
H	0.72773011066519	-2.08040744651495	3.68139373724102
H	1.76260493077854	-0.12011020451157	-0.83704257203858
H	0.83667592606586	-1.61371079892165	-0.76944468119050
H	0.46550225753028	-0.42715021212947	-2.05995924626911

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Free carbene/BP86/6-311G(d)/BSS state/130 degrees Constrained Optimization

C	0.08297719222738	-1.26938535732986	3.38664952735071
C	-1.35623894849481	-1.40583885123258	3.86196268928962
C	0.62559089864302	-0.68237161311664	-0.98920848864119
C	-0.25102549167222	0.00476727201268	-0.03646126645718
C	0.01668786317716	0.06166700568163	1.38246927174857
O	-0.00159034943095	1.10607473070768	2.02885468299261
O	0.14915893591566	-1.19634753645318	1.92756652024278
H	-1.84593975932476	-2.27379458940145	3.39521638529527
H	-1.38127004280585	-1.54313929373092	4.95526613043499
H	-1.93643374699715	-0.50312051079160	3.62127298549239
H	0.56634339985711	-0.37500924574708	3.80385532292255
H	0.68324169558445	-2.15626500990766	3.63427358269768
H	1.65001176837558	-0.25252139747628	-1.00131013762876
H	0.76561936639053	-1.72321514520676	-0.62587370735295
H	0.24057384255482	-0.70332332200799	-2.01926336638710

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Free carbene/BP86/6-311G(d)/BSS state/140 degrees Constrained Optimization

C	0.07822959732702	-1.29646824175035	3.37430984142177
C	-1.36159475725867	-1.39605584144941	3.85844721885572
C	0.50790153226049	-0.80073411969343	-0.98285120185732
C	-0.22884529846135	0.03315068391960	-0.03024161628983
C	0.02091850234164	0.07350401120378	1.39510695328334
O	0.00156293372769	1.09906004410559	2.06957577152153
O	0.13959625606186	-1.19971793562843	1.91784270776877
H	-1.88165989912404	-2.24024911208299	3.38094163023026
H	-1.38238789306038	-1.55202372662404	4.94931751640401
H	-1.91424294667384	-0.47126575227833	3.63820244496099
H	0.59022115817936	-0.42417294135757	3.80432628575853
H	0.65148104137353	-2.20613767471483	3.60279716800036
H	1.55626179001637	-0.45063983331016	-1.10000417092410
H	0.59428214323215	-1.82723918278400	-0.56996775891875
H	0.04965212005815	-0.83977325255542	-1.98253265821528

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Free carbene/BP86/6-311G(d)/BSS state/150 degrees Constrained Optimization

C	0.07230217195250	-1.31531397131332	3.36639333094568
C	-1.36463094578633	-1.38996006054519	3.86442051758751
C	0.38000426434552	-0.89057175240235	-0.98448132566359
C	-0.20086036943905	0.05479195725495	-0.02977850608102
C	0.01273897190763	0.07642990424336	1.40260070652336
O	-0.01727409578776	1.08933892630268	2.09555452706696
O	0.12340864031355	-1.20536103074370	1.91159317286974
H	-1.90674843309492	-2.21876336871461	3.38434442537592
H	-1.37734150683574	-1.55652796034360	4.95385884115764
H	-1.89966346250731	-0.45164890316539	3.65896497167257
H	0.60477247329331	-0.45719144976752	3.80051204400484
H	0.62861423039365	-2.23881918362522	3.58116679159245
H	1.45568895007879	-0.67244170516392	-1.15932488150315

H 0.35403835503453 -1.91334019624696 -0.55670142907602
H -0.12301669286836 -0.88559196076920 -1.96385305447292

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Free carbene/BP86/6-311G(d)/BSS state/160 degrees Constrained Optimization

C 0.06574509095055 -1.32840028861023 3.36159746302358
C -1.36657163161244 -1.38721243722280 3.87521261641265
C 0.24010005822515 -0.95303959293120 -0.99138343330958
C -0.16990157057574 0.06987352386192 -0.02964848629105
C 0.00057787503561 0.07651265665598 1.40773327110195
O -0.04068345087868 1.08094231137594 2.11266337926451
O 0.10416113691763 -1.21092920597516 1.90782731958226
H -1.92446093410216 -2.20651477241332 3.39675519543556
H -1.36987645024678 -1.55951028057046 4.96384674649069
H -1.89109206255343 -0.44080716801730 3.68049418184771
H 0.61282329458002 -0.47906084682964 3.79538019258171
H 0.61231491577884 -2.26012237529418 3.56608088571162
H 1.33134678077146 -0.89945074976525 -1.19358222752536
H 0.06287695776728 -1.96189509900691 -0.56750809702689
H -0.27704306205731 -0.86636283925740 -1.96019887529937

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Free carbene/BP86/6-311G(d)/BSS state/170 degrees Constrained Optimization

C 0.06085222923757 -1.33754239351963 3.35878653398307
C -1.36636158335909 -1.38797322045147 3.88740696618177
C 0.08620656613249 -0.98747093402664 -1.00019345861904
C -0.14137464724155 0.08100474720283 -0.02855445998101
C -0.01003573508420 0.07577978467514 1.41160181620591
O -0.05748136389541 1.07531747781472 2.12331608525074
O 0.08536615433886 -1.21500380695058 1.90533777430762
H -1.93506392338427 -2.20194882972035 3.41250736373459
H -1.35953263009551 -1.56366962519476 4.97551277504304
H -1.88556871107304 -0.43705366756726 3.70093863246561
H 0.61729655846823 -0.49275866612413 3.79000395625552
H 0.60323720450170 -2.27355520336875 3.55474412680608
H 1.17011139449779 -1.12895231574675 -1.19767554836551
H -0.27945436388608 -1.95344400873833 -0.59791061652424
H -0.39912717815750 -0.79384629128403 -1.97055181474415

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Free carbene/BP86/6-311G(d)/BSS state/180 degrees Constrained Optimization

C -0.00280730429988 -1.38073182627172 3.39831832057413
C -1.41808011332318 -1.33108842536908 3.95884150701658
C 0.00650994520857 -0.98337644619271 -1.08731578526124
C 0.00006162782015 -0.02113479135811 0.00461785517630
C -0.00877056417983 -0.00360988390462 1.42709453579552
O -0.01273577610055 1.01376362713430 2.12249940390772
O -0.00261759594679 -1.29337791641080 1.94411963579269
H -2.04650224473173 -2.11712571236041 3.51282523788026
H -1.39788784068726 -1.48574322420463 5.05015413021120
H -1.87996428029715 -0.35318511028966 3.76208711719506
H 0.61219477093358 -0.56178448034662 3.80004852023667
H 0.48614453143714 -2.34322352551183 3.60761136886723
H 0.91445277490803 -0.89038683195384 -1.71401152591336
H -0.03229163803971 -2.01892212026748 -0.69379984973206
H -0.85506918770141 -0.84392654069278 -1.76782033974671

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Free carbene/BP86/6-311G(d)/BSS state/190 degrees Constrained Optimization

C -0.04190744876212 -1.40301207772533 3.34393982485936
C -1.45715815275232 -1.31238306864941 3.89812167694682
C 0.04952406219435 -0.99250054444170 -1.00459968941268
C 0.22617444473615 0.06875574325881 -0.01422781664995
C 0.04108526104271 0.03774006870253 1.41948651106861
O 0.04619122392413 1.02614265894908 2.14864172849776
O -0.03092631923911 -1.26207750048586 1.89246365902355
H -2.11523611158594 -2.05528677598909 3.42203756584095
H -1.44958914866013 -1.50670730444648 4.98311608851229

H	-1.87515030933769	-0.30926019039507	3.73376000624155
H	0.60409664395830	-0.62363304456365	3.77523133044874
H	0.40498195638302	-2.39193813946402	3.52075806816182
H	0.55316451839196	-0.77402483298003	-1.96007637483100
H	0.43218579744232	-1.95246653890639	-0.60370256029340
H	-1.02479931273563	-1.16320166086340	-1.22967988641442

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Free carbene/BP86/6-311G(d)/BSS state/200 degrees Constrained Optimization

C	-0.02232432347569	-1.37745488889441	3.35755908970091
C	-1.45251266726151	-1.33652885202953	3.87820431577269
C	0.03152589037517	-0.99399724019212	-0.99481385728788
C	0.32722060030269	0.04641708590570	-0.00982958781978
C	0.06259146684864	0.03338906959039	1.41224789335123
O	0.00513434009545	1.03324923191522	2.12333555456400
O	0.01504154534005	-1.26032175261337	1.90462531389852
H	-2.06834024330844	-2.11427341715207	3.40122457954851
H	-1.46200874874856	-1.51153865610515	4.96648161550656
H	-1.90727945288119	-0.35459671304440	3.68594007484061
H	0.57999648940054	-0.56370373262518	3.78895957505124
H	0.46161209049493	-2.34322203480113	3.56258494445817
H	0.59680465018378	-0.87405905221210	-1.93251032549735
H	0.24313965385444	-1.99190790221183	-0.56077814509160
H	-1.04796418622031	-1.00530435353004	-1.25796090899584

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Free carbene/BP86/6-311G(d)/BSS state/210 degrees Constrained Optimization

6	-0.007252000	-1.354049000	3.375462000
6	-1.449916000	-1.358673000	3.861713000
6	0.015558000	-0.989497000	-0.989279000
6	0.431244000	0.008501000	-0.002156000
6	0.088298000	0.016873000	1.403473000
8	-0.029162000	1.030660000	2.086779000
8	0.059055000	-1.266112000	1.921067000
1	-2.023436000	-2.170240000	3.388345000
1	-1.478565000	-1.510569000	4.953134000
1	-1.937632000	-0.399782000	3.636738000
1	0.551887000	-0.507467000	3.802004000
1	0.509707000	-2.294861000	3.613089000
1	0.597955000	-0.948889000	-1.922621000
1	0.090918000	-2.002770000	-0.544861000
1	-1.056022000	-0.866978000	-1.257616000

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Free carbene/BP86/6-311G(d)/BSS state/220 degrees Constrained Optimization

6	0.003871000	-1.332825000	3.398796000
6	-1.449054000	-1.376683000	3.850592000
6	-0.000713000	-0.977810000	-0.991460000
6	0.530798000	-0.047637000	0.007859000
6	0.119766000	-0.014300000	1.393614000
8	-0.051915000	1.017145000	2.038212000
8	0.101477000	-1.281300000	1.943483000
1	-1.981762000	-2.220648000	3.386273000
1	-1.498986000	-1.500836000	4.944764000
1	-1.964676000	-0.442287000	3.587868000
1	0.522023000	-0.455259000	3.814316000
1	0.548512000	-2.247283000	3.674198000
1	0.564757000	-0.983700000	-1.935295000
1	-0.019071000	-1.999368000	-0.557971000
1	-1.062391000	-0.751062000	-1.229980000

15

Free carbene/BP86/6-311G(d)/BSS state/230 degrees Constrained Optimization

C	0.01083299753056	-1.31512541822348	3.42904106169176
C	-1.45143957658858	-1.38777572621184	3.84473892730409
C	-0.02252146083101	-0.95485628922397	-1.00329718924248
C	0.62117103625719	-0.12260957882434	0.01735805673594
C	0.16279659495281	-0.06502875524449	1.38470035329982

O	-0.04767368160041	0.99046613634994	1.97865069492952
O	0.14293111302970	-1.30867626874589	1.97416876147808
H	-1.94754776407170	-2.26097787635237	3.39418907804965
H	-1.52716205106853	-1.47895765388661	4.94069322645669
H	-1.98678158418557	-0.47775503908745	3.53900692983494
H	0.49234734034722	-0.40918966558996	3.82701820060675
H	0.57495352342896	-2.20296206614463	3.74835830860412
H	0.49191363258453	-0.95189251259017	-1.97535909225795
H	-0.06551267384006	-1.99399303496688	-0.61133496652491
H	-1.08567034094510	-0.67451945925785	-1.16266221896600

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Free carbene/BP86/6-311G(d)/BSS state/240 degrees Constrained Optimization

C	0.01247206605447	-1.30696138338143	3.46634873461066
C	-1.45916309333139	-1.37857029821103	3.84562430617980
C	-0.05806418742038	-0.91306978632860	-1.02428105519901
C	0.69527481822318	-0.21667431994793	0.02368358609544
C	0.21578314037264	-0.14740263002923	1.37766876982699
O	-0.01082949253127	0.93948623734108	1.91170628500021
O	0.18354717552533	-1.35867905666767	2.01428735704083
H	-1.93496315331577	-2.27312166178100	3.41553637835609
H	-1.56426432331450	-1.42883049341750	4.94176657502211
H	-1.99504003309879	-0.48648806846517	3.49141523309352
H	0.47651480256582	-0.38178183525371	3.83939464266282
H	0.57656705650544	-2.17539662263767	3.83480601425881
H	0.35540777418966	-0.79667712568849	-2.03667154690115
H	0.01590683667103	-1.98899000931823	-0.74336266419657
H	-1.14651228209544	-0.70069615421341	-1.03265248385052

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Free carbene/BP86/6-311G(d)/BSS state/250 degrees Constrained Optimization

C	0.01213762521220	-1.28930768710865	3.51519254738904
C	-1.46915711486936	-1.36644709974495	3.85156508677236
C	-0.08439543380480	-0.87375560540496	-1.04566922731237
C	0.75220200191007	-0.32824160443775	0.02815279834076
C	0.26315983601100	-0.26123566246020	1.37010870976626
O	0.01865735760984	0.86366211417085	1.82250521064734
O	0.23145993118097	-1.42418690620246	2.07292816286048
H	-1.91569581412101	-2.29256944423599	3.45861429569454
H	-1.60930838417168	-1.35634468287505	4.94483947701511
H	-2.00907376370134	-0.50620794896440	3.43059012867151
H	0.45057436278677	-0.33672030317914	3.84723959785935
H	0.57875759651828	-2.12437548650271	3.95032993575908
H	0.26641772522887	-0.64268927542780	-2.06248792313407
H	0.05236440577746	-1.97267228297255	-0.89934593564647
H	-1.17546322656725	-0.70276133265426	-0.95929273268290

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Free carbene/BP86/6-311G(d)/BSS state/260 degrees Constrained Optimization

C	0.01484691317349	-1.26945890519452	3.56781480422705
C	-1.47305973649051	-1.35063596849587	3.86962510353149
C	-0.11300390065778	-0.82109328802885	-1.06656880800710
C	0.78915530126098	-0.45246680719328	0.02932290894453
C	0.30214095236823	-0.42698276070104	1.35765912869891
O	0.04267567466277	0.74328479083439	1.69854867004733
O	0.27830019210358	-1.51857652628180	2.14556376411400
H	-1.89024911602407	-2.31494783360802	3.54184714305265
H	-1.64344215769023	-1.25555262446693	4.95438754408195
H	-2.01877797169891	-0.53937979207812	3.36658845289071
H	0.42910989017603	-0.28567166187933	3.83221596850236
H	0.58492219542464	-2.05497748325168	4.08276098767276
H	0.18936590512411	-0.44623666211314	-2.05606692716886
H	0.07196531041946	-1.92460939782797	-1.09168181848310
H	-1.20131234715178	-0.69654828771385	-0.90674679010466

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Free carbene/BP86/6-311G(d)/BSS state/270 degrees Constrained Optimization

C	0.02581311500723	-1.24677501833485	3.60288972141189
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C	-1.46383802571156	-1.35385950923485	3.88834931345473
C	-0.12214608032960	-0.79540396486120	-1.08884885928656
C	0.80186407627176	-0.57657863387712	0.03003297808690
C	0.31409117751059	-0.52817614931663	1.35251404648412
O	0.02311966771685	0.65752000970292	1.61801527155540
O	0.31975058224919	-1.56842871442455	2.20129571664184
H	-1.84855853192928	-2.34659837957947	3.60942894951237
H	-1.65282761648823	-1.20379212544685	4.96372353244811
H	-2.02538172043873	-0.58815386735888	3.33385611661176
H	0.40946507381433	-0.23913072292156	3.81841894059702
H	0.60859216209177	-1.98607910260403	4.16930402808188
H	0.21519687452795	-0.36243881897714	-2.04305609427830
H	-0.05113467977598	-1.90261257054516	-1.22254951145727
H	-1.19136896951632	-0.57334564022064	-0.90810401786386

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Free carbene/BP86/6-311G(d)/BSS state/280 degrees Constrained Optimization

C	0.03662354099758	-1.22821570198837	3.62892504633042
C	-1.45171537314966	-1.35919323466537	3.91197344945947
C	-0.12842040651906	-0.77054821856363	-1.11140939797158
C	0.79220816488137	-0.69967901788393	0.02814748056261
C	0.30660661572717	-0.61121537354919	1.34719298611199
O	-0.01355932512722	0.58026231442610	1.55416024076107
O	0.34769283281018	-1.60634778977737	2.24552597610411
H	-1.81005280309438	-2.37286149794468	3.67670735989692
H	-1.65032444313238	-1.16535510537499	4.97858185014801
H	-2.02961209617557	-0.63384456655270	3.32114817819619
H	0.39537473938297	-0.20338148636981	3.80109187085825
H	0.63325597999063	-1.92724289377785	4.23082936740022
H	0.25683496632433	-0.28206344924674	-2.02008825887281
H	-0.14604204212392	-1.86062398999607	-1.35257339078659
H	-1.17623324579203	-0.47354319673541	-0.91494262619829

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Free carbene/BP86/6-311G(d)/BSS state/290 degrees Constrained Optimization

C	0.05343574987751	-1.20418774696262	3.64269245517442
C	-1.43080120035502	-1.40261822659109	3.91140969151627
C	-0.12542235894371	-0.77507898440906	-1.13541263335436
C	0.76556413463778	-0.78849437453886	0.02847218407405
C	0.28979326705430	-0.57763342295192	1.35292637504601
O	-0.07998030619500	0.58867507053342	1.57186732565803
O	0.39731983351244	-1.56588269234383	2.26576065953251
H	-1.74039153327610	-2.43132475072276	3.67201265588728
H	-1.64888403882901	-1.21894047991558	4.97602607117365
H	-2.03508739288975	-0.70363562249677	3.31526503457002
H	0.36243877391499	-0.16422641941697	3.81996630590159
H	0.67374008522770	-1.87616914732702	4.25165374307034
H	0.36226850598836	-0.42294018609737	-2.05794409792054
H	-0.40512152449918	-1.83746749388145	-1.32348158210224
H	-1.07623489022530	-0.23392873087812	-0.96594405622703

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Free carbene/BP86/6-311G(d)/BSS state/300 degrees Constrained Optimization

C	0.06718221561814	-1.18533204813438	3.65738361108105
C	-1.41029611100183	-1.43455555643134	3.92379959148921
C	-0.12714650795627	-0.76529701696106	-1.15957458642924
C	0.72086456054046	-0.87540659810846	0.029797272409762
C	0.26416115509155	-0.58540626854249	1.35393430827871
O	-0.14631647499726	0.56497442554924	1.56574635121795
O	0.43115550705335	-1.55094280457096	2.28870545706453
H	-1.68076627656146	-2.47707935929425	3.69704430147897
H	-1.63938856350635	-1.24481848052938	4.98501521748615
H	-2.03749650768544	-0.76622840765246	3.31630064165120
H	0.33656820984227	-0.13254124575493	3.82317130116485
H	0.70833608414640	-1.82658558526211	4.27787459487845
H	0.43125713994599	-0.49933345990203	-2.07101355264325
H	-0.57882293302682	-1.76475474340734	-1.35121031251076
H	-0.97665440150270	-0.07054605899804	-1.011170451630541

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Free carbene/BP86/6-311G(d)/BSS state/310 degrees Constrained Optimization

C	0.07505792114588	-1.16943179277918	3.67031360464485
C	-1.39732768152548	-1.44183190217377	3.94485006183390
C	-0.12191149397137	-0.76308602663010	-1.18551005606370
C	0.66406102462209	-0.97316419554467	0.03161791192712
C	0.23312283862100	-0.61068736143107	1.35217355079895
O	-0.20083920004237	0.53069300192279	1.55356381427293
O	0.44405178923458	-1.55074558495491	2.30923638020101
H	-1.64815560776419	-2.49315936284415	3.73692326145890
H	-1.62806608336214	-1.23763135320285	5.00298722060431
H	-2.03834015378926	-0.79634086266029	3.32719818327941
H	0.32417426775291	-0.10896693080989	3.81853230655188
H	0.72862991915263	-1.78793804303568	4.30097889589876
H	0.49925681530909	-0.57266343141210	-2.07538193357972
H	-0.70444617173507	-1.68565133332524	-1.40290590886157
H	-0.86663107864829	0.04675197088110	-1.05930716096705

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Free carbene/BP86/6-311G(d)/BSS state/320 degrees Constrained Optimization

C	0.08035823341710	-1.15362670908247	3.67923743236716
C	-1.38307677329091	-1.45808104852000	3.96929831575482
C	-0.11142971123574	-0.75535800203178	-1.21067033922812
C	0.59972277923918	-1.05426047039784	0.03328171804101
C	0.19249004839688	-0.63248436566770	1.34824977840778
O	-0.27073835387642	0.49700981820275	1.54188040107674
O	0.44910815270326	-1.54779321490299	2.32289028797565
H	-1.60871131149203	-2.51880025398091	3.78129939358075
H	-1.61093217446978	-1.24143534026388	5.02558910384767
H	-2.04419729407079	-0.83936766387251	3.34556855216934
H	0.30262348225300	-0.08451505229872	3.80749423897265
H	0.75357053589838	-1.74503431415198	4.31521205591740
H	0.55986304478932	-0.66739157389055	-2.08009027264497
H	-0.82429363065633	-1.57615653521151	-1.44309784757370
H	-0.72171992260512	0.16344151807008	-1.11087268666421

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Free carbene/BP86/6-311G(d)/BSS state/330 degrees Constrained Optimization

C	0.08623051637581	-1.14326384787925	3.68379448342468
C	-1.36641917241544	-1.46317877002599	4.01086237309300
C	-0.09732387920451	-0.74230355604349	-1.24222935435602
C	0.51512035562785	-1.12556026818367	0.03005980968354
C	0.13340385004265	-0.66685628898233	1.34128391812039
O	-0.35631057773937	0.45222016187735	1.52879697094064
O	0.43254760375883	-1.55757990883241	2.32895411789895
H	-1.57978912826814	-2.53051384075638	3.84771587090125
H	-1.57556164743736	-1.22923038619284	5.06731758178870
H	-2.04919631736910	-0.86629719389647	3.38931370292226
H	0.29423581038480	-0.06847806639455	3.78809033730190
H	0.78081930181152	-1.71255087806135	4.31708584483914
H	0.63127236847091	-0.69673718163765	-2.06859796343180
H	-0.86171251714708	-1.49111061227806	-1.54076602310386
H	-0.62467946189137	0.22758742928707	-1.15641153802279

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Free carbene/BP86/6-311G(d)/BSS state/340 degrees Constrained Optimization

C	0.08739567962699	-1.12588019661162	3.68431695890968
C	-1.34720974439607	-1.48541010251269	4.04860512851215
C	-0.07579173876960	-0.72559392388315	-1.26837402526442
C	0.43500625070023	-1.17728976933577	0.02586464696728
C	0.06932423587158	-0.69397018899105	1.33294670109142
O	-0.46307610057940	0.40665807007682	1.51360512475125
O	0.41817836071442	-1.55594567851840	2.33131881871497
H	-1.52903612228508	-2.56211545631419	3.91099859991955
H	-1.54167336634216	-1.23670799621195	5.10451570931138
H	-2.06126986524883	-0.92331759498289	3.42989753873200
H	0.26152295776789	-0.04274955632609	3.76348201183301

H	0.81297137172697	-1.65970522831246	4.31380390822689
H	0.67849322508135	-0.80086012737346	-2.06928126447792
H	-0.93801120821232	-1.34791897561317	-1.58821542161583
H	-0.44418683065597	0.31695351691006	-1.20821430361144

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Free carbene/BP86/6-311G(d)/BSS state/350 degrees Constrained Optimization

C	0.07919627545873	-1.08938715436352	3.68271992143536
C	-1.32306456835356	-1.53284404090867	4.07909950751846
C	-0.04433263118509	-0.70413703461616	-1.28537976867832
C	0.37645457663685	-1.21144131668278	0.02128774525547
C	0.00128133559674	-0.71898345939977	1.32274466615165
O	-0.61091630366533	0.34250954873659	1.48534758588550
O	0.41769438680719	-1.53150318021630	2.33573296977765
H	-1.43512886819364	-2.62236629640613	3.97136845372189
H	-1.51749720600602	-1.27011751623036	5.13163141834391
H	-2.08146778457303	-1.03499412330082	3.45826359511196
H	0.18199993335472	0.00474545175839	3.73270082673692
H	0.84753330416584	-1.55799733493618	4.31340587328231
H	0.63517068825383	-1.01704362833806	-2.09466957361486
H	-1.05768930062870	-1.07229224524571	-1.55070673750765
H	-0.10659673266852	0.40199912214944	-1.27827635142023

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B3LYP Scan/Melmid IPC Model/RKS/0 degrees Constrained Optimization

C	38.94473762770801	-22.88169128368541	4.92071899585690
C	37.76502001940666	-23.78196787468686	4.74979313465237
C	37.10322006895902	-24.61169468109463	5.61952381442330
N	37.08782601748744	-23.92990325678743	3.54729235087270
C	36.07384103177839	-24.81928557294626	3.73873046750542
N	36.06003852110273	-25.24741066671694	4.98098643045364
C	30.54911306175910	-24.85207679716502	2.41295212564161
C	35.57904532481329	-24.57721189570529	10.96853927118531
C	39.28063292832319	-29.85973458580626	6.32043716230134
C	33.71691162523285	-28.81676568592530	0.68713910400848
N	33.16279084207150	-25.60005384162800	5.00745576752322
N	34.60058932665695	-25.52599728827047	7.46815730130658
N	34.82915379263681	-27.71399596394511	4.10261896191004
C	32.84559401718928	-26.87143372202190	2.94017526518866
C	32.93404981975962	-23.88675252517104	6.74042198550651
C	36.27714421437361	-26.69326114290507	8.81530850252144
C	36.94033407640015	-28.86496155971773	4.55380257675449
C	30.70441605868911	-22.76264347818575	4.90691010262339
C	33.42977235546929	-22.60510386984190	9.52049806302670
C	38.73252905405503	-28.53596607642920	9.24482609346581
C	36.57197035217128	-30.01436730236641	1.69849119149985
C	32.50476780143640	-25.85937496940646	3.83391880298515
C	33.84633035563645	-24.39947520035501	7.65880862753388
C	36.75414930313519	-27.55743737845255	7.83314308887221
C	35.85621644725975	-28.54264777136341	3.74397948053303
C	31.46703666925871	-24.86548869211518	3.59986079064931
C	34.08377885334853	-23.84419493383782	8.98382660654332
C	37.94086498817117	-28.38971276245405	7.97885151588623
C	35.63405482260939	-29.08388748313169	2.41090182146301
C	31.53360743195975	-23.98546217764507	4.64691603589328
C	34.98531514761736	-24.67442994331414	9.59432017237611
C	38.16958959006845	-28.94794084625253	6.75042902005369
C	34.43451531045451	-28.57821293966296	1.98312656981853
C	32.59206720002702	-24.46763209149790	5.52239937789584
C	35.30861981694314	-25.71144093170266	8.62536194410982
C	37.09865172896844	-28.48127295479129	5.88075063213293
C	33.95984814042409	-27.70147934290853	3.04475855346562
N	36.25555928365054	-27.64780359550653	6.56239281251167
Fe	34.61309341768385	-26.72789194945938	5.84747742665122
C	34.54466350414487	-31.37007610866136	5.96353498212302
C	33.74709674844425	-31.95142571342075	4.80597792848039
C	32.15824700479983	-27.38006827971508	7.23647655763427
C	33.41154006845701	-27.85262261948882	6.56064948213887

C	33.41457204613522	-29.36968605772089	6.56015951300720
O	32.51862447938584	-30.03701078267174	7.04405033255797
O	34.48894947833277	-29.92966385260000	5.98121691493022
H	29.98399199382444	-22.58518914800350	4.10218472246800
H	31.32538318814354	-21.86121397843355	4.99585277593611
H	30.13421760740011	-22.85102516085576	5.84149790064718
H	31.10379266534612	-24.77368105286391	1.46803271063422
H	29.94768936504365	-25.76921827355153	2.35456720430797
H	29.85328632956231	-24.00828756063322	2.45302383020836
H	33.53375709686480	-27.88012113688090	0.14353227689413
H	34.29190113832540	-29.47093029656473	0.02415654707766
H	32.73869814809993	-29.28978366299963	0.84605048324847
H	36.21749029013318	-30.24529320403707	0.68906792939161
H	37.57705308396402	-29.58222738293909	1.60244600343165
H	36.68470976390518	-30.96810842254416	2.23137799749762
H	33.79369796916478	-22.36312706984059	10.52394775975914
H	32.33896175696556	-22.71614176372768	9.58619366934031
H	33.62495218005007	-21.73409715634500	8.88064796505459
H	36.67240861580670	-24.47736843628688	10.93337208180638
H	35.35920292344820	-25.46948636051328	11.56979702944792
H	39.57880752936330	-29.21700246394820	9.11158271939363
H	39.13671697299856	-27.57368700223072	9.58768954428790
H	38.11776493584926	-28.93412693855378	10.06322632394408
H	38.90268845125347	-30.83081821863682	5.97324226305878
H	39.85926777658943	-29.42769012679287	5.49274649082732
H	39.97980020498191	-30.05743654606671	7.13913010624891
H	35.18905603817445	-23.71229696913448	11.51392623776636
H	39.77809284280435	-23.16064619872739	4.26174362382439
H	38.69794440303712	-21.83093686414206	4.71617043556515
H	39.30564330597816	-22.94092877645756	5.95166319950358
H	34.07512914472833	-31.51993644108740	3.85745133267911
H	33.8888666861096	-33.03625771685256	4.76095436387102
H	32.68200113385002	-31.75196693608494	4.93196166449310
H	34.18402634254725	-31.75146621396785	6.92099391831815
H	35.60846587068234	-31.59072651841277	5.86440327442957
H	32.16054672110149	-26.31804535269552	7.45397922217146
H	31.30316769692433	-27.59027254499407	6.57732897813766
H	31.96037879511290	-27.94799293079019	8.15077751086477
H	37.30634125859834	-23.46058633988376	2.68023964808091
H	37.31030767600767	-24.79155773118993	6.66416915879235
H	35.38516340496714	-25.12117305074196	2.96322126203896
H	32.24188433171602	-26.96325581522539	2.04278684374217
H	36.76667646825214	-26.72556206418619	9.78359379391310
H	37.69476915071250	-29.52401559996368	4.13516358491117
H	32.39960596971485	-22.98603221607479	7.02530165351016

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B3LYP Scan/Melmid IPC Model/RKS/10 degrees Constrained Optimization

C	38.95467003725339	-22.91143918201990	4.90558140135643
C	37.76756583325848	-23.80303593550188	4.74053749234787
C	37.09605152029950	-24.61755177377555	5.61711934631385
N	37.09352990929976	-23.95915272800679	3.53729094084519
C	36.07204493621345	-24.83853951016582	3.73487234978781
N	36.05049677743988	-25.25255238413139	4.98181676498882
C	30.54656443517053	-24.84175002059941	2.42088869872700
C	35.58216283486420	-24.57326602943125	10.97468472056905
C	39.26428017127564	-29.87084884202467	6.32600357810771
C	33.70140558940022	-28.81423344099577	0.69470558419812
N	33.15527929410632	-25.59786364369378	5.01794575121355
N	34.59538361444571	-25.52467615353451	7.47723127931053
N	34.81311351869981	-27.72244345082257	4.11394748694456
C	32.83453493529968	-26.86921016453732	2.95038412357935
C	32.92924649033782	-23.88449191237746	6.75148160256572
C	36.27439818858269	-26.69134736783501	8.82112272976622
C	36.92669510157434	-28.87000206176170	4.56119002876839
C	30.70407726932566	-22.75462172953000	4.91656522411755
C	33.43244279198500	-22.59974210315177	9.52886180773208
C	38.72291777263838	-28.54296359745151	9.24987822000961

C	36.55677399160702	-30.01349137497983	1.70117534259245
C	32.49725050648029	-25.85566187664238	3.84388223463559
C	33.84254442048326	-24.39711768442673	7.66857468358897
C	36.74989285917895	-27.55461132970754	7.83755724314778
C	35.84015168080979	-28.55002498563523	3.75309857735442
C	31.46243452138061	-24.85892536110357	3.60933623626321
C	34.08322889309590	-23.84071462759995	8.99261528241920
C	37.93308516313959	-28.39188947553631	7.98335479117760
C	35.61827270802076	-29.08681926344806	2.41797138763653
C	31.52975626849536	-23.97998048096129	4.65726246753378
C	34.98517775746992	-24.67129331162068	9.60194830654754
C	38.15926886083307	-28.95140577104091	6.75518533110757
C	34.41919742107413	-28.57885542245939	1.99110019020368
C	32.58606682009055	-24.46513891664313	5.53356559247102
C	35.30563832633000	-25.70931686512705	8.63291953347088
C	37.09015488769750	-28.48045256098731	5.88557558943554
C	33.94481108433965	-27.70474285838866	3.05479558228862
N	36.25142250281228	-27.64226279553495	6.56680528999739
Fe	34.60540498572765	-26.72632416794567	5.85591990202900
C	34.54137640157989	-31.37264234372617	6.01454950804539
C	33.90114925659705	-31.89762846451594	4.73835784338667
C	32.15579996229828	-27.38571584993787	7.25602426024410
C	33.40095089124750	-27.85252362944870	6.56100099741501
C	33.36250022708227	-29.36445590477919	6.46880484110953
O	32.37526137344804	-30.02227754131035	6.74241666488368
O	34.51640977718473	-29.93214828072717	6.08326853689313
H	29.98433236278271	-22.57541690175029	4.11162523794166
H	31.32781951419521	-21.85503928390722	5.00500187226189
H	30.13349106345996	-22.84070340225150	5.85110983765662
H	31.10321257226117	-24.76397642142415	1.47706425194514
H	29.94257356849015	-25.75704576950060	2.36055842253166
H	29.85321714622650	-23.99590447590598	2.46054788110737
H	33.50984277356363	-27.87546619905570	0.15783605262489
H	34.28024107065254	-29.45950797251925	0.02637432549577
H	32.72733731828426	-29.29615290324355	0.85245876513311
H	36.20514775485625	-30.23506764924746	0.68866747040581
H	37.56292169674352	-29.58238488254175	1.61236605945023
H	36.66624531433576	-30.97236158616828	2.22558688396352
H	33.79726096045635	-22.35811417364917	10.53207501704835
H	32.34136041190126	-22.70786285070264	9.59481450955237
H	33.62971673014282	-21.72960551332577	8.88844556482485
H	36.67551599748457	-24.47434969307704	10.93692427029905
H	35.36305429927295	-25.46482807629701	11.57730861068043
H	39.56679255752595	-29.22695649836887	9.11649043050356
H	39.13032854646320	-27.58277741810962	9.59478290547778
H	38.10582189179744	-28.94016519512589	10.06703181582942
H	38.87946084325966	-30.83941308981677	5.97931088888770
H	39.84612758397280	-29.44353212976603	5.49811071935505
H	39.96181303845967	-30.07298908519113	7.14500729834861
H	35.19407655006887	-23.70755140702687	11.52018166591243
H	39.78801030862991	-23.20585838451593	4.25334528732662
H	38.71847890792672	-21.86094715995170	4.68769493673046
H	39.31095645717873	-22.96191814656088	5.93860052210874
H	34.35851258265074	-31.43781476725031	3.85946550947079
H	34.03622844931125	-32.98238648801370	4.67301806225977
H	32.83168909047684	-31.68474131840632	4.72763114914811
H	34.04358323425767	-31.77813579348264	6.89804224327412
H	35.60386537769037	-31.61659457667858	6.05589412392613
H	32.17488396485044	-26.33203535893715	7.51083444014279
H	31.29926957401781	-27.56347736851220	6.59069765152100
H	31.94843926511710	-27.97998058147167	8.15258203185608
H	37.31915987249214	-23.50180255522858	2.66568376710748
H	37.29838017877237	-24.78796601460278	6.66426347921325
H	35.38414726021099	-25.14409906972011	2.96010624466159
H	32.23090330203334	-26.95783195933791	2.05263344130233
H	36.76479608091594	-26.72481984658585	9.78893821601710
H	37.67902039934075	-29.53152025142384	4.14267631526333
H	32.39593851432583	-22.98308069876502	7.03630017430507

B3LYP Scan/Melmid IPC Model/RKS/20 degrees Constrained Optimization

C	38.92919270393942	-22.88499824139029	4.90988389980461
C	37.75461623172797	-23.79272054022417	4.74278569044840
C	37.08513077839864	-24.60758981248073	5.62059668490988
N	37.09186621411651	-23.96581337594404	3.53561585531359
C	36.07842303302088	-24.85463660236947	3.73215950706327
N	36.05122432768180	-25.25872165915547	4.98235352960259
C	30.54775861241166	-24.83762900945766	2.42790277086828
C	35.61227877487115	-24.56018661577519	10.96818250797815
C	39.25222679112711	-29.89392950926729	6.32856377542820
C	33.71310207972343	-28.78996329502122	0.68168939897483
N	33.15869160884768	-25.595044436071667	5.02198286636689
N	34.59975161035711	-25.52647806505984	7.48179040743472
N	34.80825428731958	-27.73243632046660	4.11735071600606
C	32.84165392840197	-26.85850606355466	2.94805071136839
C	32.92858680786295	-23.88873037879060	6.76182763496542
C	36.28877553581793	-26.68655410523131	8.81851918514987
C	36.91269677088896	-28.89363560680092	4.56862283797280
C	30.69336761862467	-22.76394369161175	4.93543570167544
C	33.44763374766436	-22.59559411334022	9.53201817549411
C	38.73608951396158	-28.53810560237272	9.24392227186499
C	36.55302399832140	-30.01425870327505	1.69604851424562
C	32.50214476064237	-25.85003729787964	3.84628295748011
C	33.84726959610715	-24.39866413149853	7.67475158353199
C	36.75680620420108	-27.55523912811001	7.83645794800618
C	35.83144406215782	-28.56491503482543	3.75684679060378
C	31.46334919969224	-24.85645549321720	3.61649775995584
C	34.09604006130935	-23.83774965151262	8.99555085235810
C	37.93725106188779	-28.39634241853048	7.98191253244908
C	35.61516082979026	-29.08915910692409	2.41590812384296
C	31.52563775719154	-23.98333544356694	4.66951672340489
C	35.00378524199332	-24.66473827916100	9.60093183803263
C	38.15287283985347	-28.96764593749378	6.75747593412446
C	34.42307341509371	-28.56870885286269	1.98471123383862
C	32.58443550748057	-24.46788496075978	5.54327695753778
C	35.31805711345744	-25.70602466277411	8.63309497162567
C	37.08138392937192	-28.49773995782350	5.89013300477815
C	33.94711102148068	-27.70045721494054	3.05216151472701
N	36.25119241411215	-27.64902677237381	6.56882768761742
Fe	34.60785772781100	-26.72772913508108	5.85925094737641
C	34.44544513431624	-31.40694477482842	6.09149976921945
C	34.00610915431616	-31.90718040148594	4.72409822987959
C	32.16156947788026	-27.38763939757627	7.27248312545046
C	33.39219233811802	-27.85030526898077	6.54837617429801
C	33.29698412463633	-29.34789428899715	6.35403305157173
O	32.24425345681144	-29.95542394299322	6.41042105998558
O	34.47543499863878	-29.96542890067450	6.17108952057511
H	29.96930589409097	-22.58731145484640	4.13380331023711
H	31.31155726963306	-21.86049838796349	5.02375890780729
H	30.12702656329093	-22.85623552268875	5.87194690050587
H	31.10422004317228	-24.74856950737573	1.48492136590978
H	29.95114226685333	-25.75722282539152	2.36072934218656
H	29.84786857416505	-23.99750367937299	2.47342159542513
H	33.51556217421894	-27.84484003078241	0.15854619784878
H	34.30050643926032	-29.41992957200215	0.00622159778201
H	32.74273473458417	-29.28305834336476	0.82779360882080
H	36.21602203306458	-30.20952467524006	0.67321534646421
H	37.56621145756448	-29.59530166160552	1.63378855752415
H	36.64075956810758	-30.98606747500609	2.20062977657847
H	33.81740110289543	-22.35136845021034	10.53279589960829
H	32.356915764449813	-22.70387803335690	9.60370098969841
H	33.64129644535325	-21.72697081733223	8.88844900514206
H	36.70480979063169	-24.45635750145539	10.92048049717995
H	35.40283619617743	-25.45102522085654	11.57530438687774
H	39.57581404210173	-29.22729444457905	9.11101113549309
H	39.15081452976930	-27.57632150863615	9.57554122432028

H	38.12382382364887	-28.92385738544949	10.07013374503401
H	38.86148978809263	-30.86047014421469	5.98313103181081
H	39.83597599443755	-29.47074743401992	5.49980038971206
H	39.94934984124865	-30.09898187928366	7.14722923281915
H	35.22504400232011	-23.69471442562536	11.51469581200336
H	39.76987905407062	-23.17159024506060	4.26363404104494
H	38.68029520154543	-21.83881334118591	4.68537919566584
H	39.28046096393775	-22.92546836657105	5.94504668800664
H	34.62947445740252	-31.48002042229328	3.93593495363715
H	34.09377340563924	-32.99803667730322	4.68264709035379
H	32.96730229439262	-31.63794642657504	4.53285865186891
H	33.78595327153946	-31.78771307362959	6.87476515511779
H	35.47255325804959	-31.70062435802985	6.31261056286982
H	32.19851630538844	-26.34322545424530	7.56069440731107
H	31.29612142753285	-27.54041948002311	6.61451233737880
H	31.96075827968838	-28.00455332272211	8.15686821515331
H	37.31928460242275	-23.51274986623145	2.66223389213254
H	37.28080481434459	-24.76720032218170	6.67068905692247
H	35.39913712340264	-25.17270818405575	2.95485910334673
H	32.24101178107362	-26.94028561093478	2.04767255773050
H	36.78581607483472	-26.71557574182777	9.78309614532381
H	37.66017139744038	-29.56225012602055	4.15274942452522
H	32.39380852967631	-22.98895856627184	7.04906942961389

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B3LYP Scan/Melmid IPC Model/RKS/30 degrees Constrained Optimization

C	38.92859406201227	-22.88536575171243	4.89961862684336
C	37.74906517401399	-23.78641540141518	4.73154419553144
C	37.07648294885683	-24.60000696233319	5.60811458101390
N	37.08456813236512	-23.95369251332071	3.52451754857120
C	36.06703251162136	-24.83805621438109	3.71972245086713
N	36.03906932376197	-25.24480143556544	4.96913741386000
C	30.56051848565496	-24.76303437264250	2.41150914293519
C	35.60873810843842	-24.59239012347487	10.96772298047027
C	39.20319670097603	-29.93955107993613	6.29448849952585
C	33.67370092228384	-28.75195829905523	0.65695066395247
N	33.15020892785363	-25.56846877981431	5.01275654528611
N	34.59172819125695	-25.52547820378127	7.47365863264404
N	34.78789709490701	-27.71424141273145	4.09268592304871
C	32.83380827176461	-26.80914428334872	2.92474828065003
C	32.91633382849253	-23.88373545743915	6.77311746308159
C	36.28714250830311	-26.69473313295984	8.79456897677516
C	36.87726609026200	-28.90308779950388	4.53989297552427
C	30.69767124509039	-22.72526801359174	4.94857346953135
C	33.43102684198806	-22.62281687927468	9.55890127228828
C	38.71373425420631	-28.57598255353092	9.21150594336061
C	36.49000423213359	-30.02839876366220	1.67242829702574
C	32.49903586839660	-25.80564159076667	3.83065185465457
C	33.83488356522332	-24.40318415709711	7.68071182207418
C	36.74984115100346	-27.55922002979614	7.80650640720259
C	35.79770163707926	-28.56257846825197	3.73032152981723
C	31.46712623432596	-24.80338178465653	3.60640971737772
C	34.08397166141518	-23.85585833768149	9.00712836872961
C	37.91795149696918	-28.41788980916260	7.94961638899091
C	35.57128529782951	-29.08303002949658	2.38981374787784
C	31.52581164803477	-23.94512998284893	4.67171200956143
C	34.99772215240053	-24.68469789354488	9.60074228498682
C	38.12314910480502	-28.99156094388780	6.72458392097906
C	34.38896451795696	-28.54130826581408	1.95879217126629
C	32.57708332160593	-24.44596411095611	5.54532524439491
C	35.31407196430343	-25.71413593113507	8.62086860967209
C	37.05851897516134	-28.50329609532478	5.85882598169328
C	33.92705318610307	-27.66658593555396	3.02687683768729
N	36.24368113903455	-27.64170812646421	6.53842133429291
Fe	34.60175993675553	-26.71001387703071	5.83869634831577
C	34.44288524555807	-31.41830691573967	6.31079555442653
C	34.33363973096382	-31.95860291427491	4.89382817975031
C	32.14254446368437	-27.40410603301163	7.22139452094787

C	33.39198663719287	-27.84432487884657	6.51520135151455
C	33.31035703304221	-29.33420919927764	6.28158841785884
O	32.25699960218062	-29.91926461417960	6.12204341546800
O	34.49028822451930	-29.97456314192713	6.35370046686809
H	29.97673437630265	-22.53666366097638	4.14683331737847
H	31.31918977315433	-21.82530358794350	5.04878031180067
H	30.12802825399893	-22.82551736299721	5.88225571652690
H	31.12463563730835	-24.66503388705073	1.47396764511859
H	29.95847349333497	-25.67770334770807	2.32764113376708
H	29.86580175447287	-23.91893349944133	2.46299072583091
H	33.48520665321389	-27.80360215654141	0.13628731555470
H	34.25280163200606	-29.38653940607639	-0.02130678436049
H	32.69828414129586	-29.23462160276876	0.80442581749642
H	36.14614540933486	-30.22383470782324	0.65187904556346
H	37.51057446058164	-29.62861882916430	1.60427944689637
H	36.56147419644769	-30.99873410354000	2.18266059156069
H	33.80146915647529	-22.38845591283288	10.56179038380197
H	32.34087836466293	-22.73653525540654	9.63107955629602
H	33.61977939435095	-21.74594244943233	8.92509008334163
H	36.70098032591509	-24.48633017149600	10.91891335062775
H	35.40206183498261	-25.48952150586192	11.56654940131512
H	39.54782092937612	-29.27123883396633	9.07463701249923
H	39.13606288570215	-27.62035245188087	9.55109799753688
H	38.09696808278778	-28.96282518141023	10.03393810910310
H	38.79220204168251	-30.90041454937078	5.95671843415298
H	39.78978059089740	-29.53199892478009	5.45996848604264
H	39.90118214854154	-30.15309437862060	7.11025883306664
H	35.22109062825446	-23.73295923927677	11.52345395416603
H	39.76779272649189	-23.17622688878609	4.25333854840966
H	38.68562845215887	-21.83763199495747	4.67588626202339
H	39.27938457639345	-22.92867111482427	5.93482864591808
H	35.15447140189281	-31.59153660736238	4.27508626162898
H	34.37429106878524	-33.05286259489345	4.91118715861765
H	33.39050899525076	-31.65664970675239	4.43820401503813
H	33.60415784521245	-31.75919797971073	6.92167935197198
H	35.37804674978108	-31.72308598463719	6.78282138315364
H	32.16006388515166	-26.36027286903554	7.51514542945587
H	31.29384431386970	-27.57006868077518	6.54580801422734
H	31.93707230802886	-28.02587727032288	8.10257505661872
H	37.31355708448422	-23.50000247338024	2.65188457011938
H	37.27226194568016	-24.76327916215866	6.65760275082064
H	35.38545793494863	-25.15111264419437	2.94242221596705
H	32.23523212562144	-26.87770251899617	2.02185347173404
H	36.78542345603937	-26.73244898171044	9.75823859547372
H	37.61331354167933	-29.58396861148383	4.12342205375997
H	32.38058075666124	-22.98777450245019	7.07036966078227

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B3LYP Scan/Melmid IPC Model/RKS/40 degrees Constrained Optimization

C	38.91893106848244	-22.87187538429762	4.90525845807100
C	37.74369481431193	-23.77780134024966	4.73331041849387
C	37.07044299753871	-24.59278924124153	5.60801638899084
N	37.08468597939399	-23.94857767989244	3.52378752608643
C	36.06932439713105	-24.83602899442092	3.71558012375803
N	36.03759990957559	-25.24160354647091	4.96541110993877
C	30.56723570733240	-24.72704967649289	2.40572010634414
C	35.62612970572254	-24.59684480003133	10.96054809972975
C	39.17940933785017	-29.96737300967078	6.27896259879261
C	33.65561884091306	-28.73125883792736	0.64287153690114
N	33.14999300922214	-25.55257279638576	5.00733222982696
N	34.59046982808605	-25.52497729662800	7.47037940669561
N	34.77996704844502	-27.70562208573679	4.07899202654019
C	32.83784541365605	-26.77741603751774	2.90905318565323
C	32.90671168696593	-23.88599443218562	6.78370993587432
C	36.29745917394681	-26.69196579194056	8.77860861281531
C	36.85149796627218	-28.92344791439250	4.53037984976136
C	30.68606733358536	-22.71873575059383	4.96704299300798
C	33.42737805462338	-22.63559708878019	9.57301760641478

C 38.72037740124542	-28.57788488706709	9.18812681764944
C 36.44389927228579	-30.05725698335522	1.66789253428162
C 32.50320249352501	-25.77930890181386	3.82092482080789
C 33.82968770862652	-24.40701072691139	7.68590115683438
C 36.75276258770949	-27.55922853247083	7.78974528433349
C 35.77657700868689	-28.57111041389956	3.71950883162821
C 31.46971500330652	-24.77722438471141	3.60330079536758
C 34.08345525955727	-23.86321914658945	9.01292526513729
C 37.91665549272954	-28.42386301858583	7.93071637000734
C 35.54355497025239	-29.09088172739809	2.37996809813307
C 31.52084370396008	-23.93137708155104	4.67874536117921
C 35.00588204170554	-24.68870047939399	9.59765849834256
C 38.10926319170419	-29.00819498007472	6.70882420265045
C 34.37194540061848	-28.52914674782768	1.94541584394142
C 32.57119417404508	-24.43804563941760	5.55024324865561
C 35.32056539488978	-25.71376159529652	8.61255396780208
C 37.04254588782155	-28.51786086482063	5.84654842530998
C 33.92173072285441	-27.64619027377028	3.01146629021397
N 36.23892226800013	-27.64511159898252	6.52481189646708
Fe 34.60251318000638	-26.69956531480274	5.82705224432317
C 34.34779091299663	-31.43813737939123	6.40004260983561
C 34.55309219614030	-31.96894188082445	4.99079230202321
C 32.14313679017614	-27.42046471733485	7.21262841737183
C 33.39020750886514	-27.83853850791194	6.48947532713259
C 33.30118968722503	-29.31393308397271	6.19484423848647
O 32.27226031967721	-29.85124819475880	5.83821423453519
O 34.42917568881923	-29.99524246673074	6.46723245953451
H 29.96551985441297	-22.52545718257003	4.16605868681723
H 31.30249832439608	-21.81652519109745	5.07803435523879
H 30.11527736603324	-22.83202642802263	5.89854551954327
H 31.13455936861722	-24.62022250662467	1.47109265043684
H 29.96654006217889	-25.64163512482000	2.31172706679020
H 29.87150346246704	-23.88411383596281	2.46228004327120
H 33.47807050474150	-27.78065941794874	0.12245866839187
H 34.22846931816738	-29.37182880186242	-0.03507049277911
H 32.67488738025173	-29.20321738601071	0.78951286168466
H 36.11080976192199	-30.23205316099371	0.63999650216846
H 37.47747220504908	-29.68939643201223	1.61963547201376
H 36.47536005620499	-31.03397344730841	2.16977468580888
H 33.80245949205244	-22.40297718420644	10.57459755215462
H 32.33823828876368	-22.75513079216347	9.65105650524894
H 33.60787916430410	-21.75538134983622	8.94142384271952
H 36.71755933738135	-24.48620091489206	10.90416655519680
H 35.42756489193359	-25.49600971793323	11.55909529839580
H 39.55286283634364	-29.27453113909536	9.04861763718733
H 39.14588994503885	-27.62134343937824	9.52110217817817
H 38.10870186339343	-28.96074928119974	10.01622674944545
H 38.76003116627215	-30.93095528081052	5.95951394710022
H 39.75811375416090	-29.57422978890566	5.43215684797507
H 39.88607233692196	-30.17306371925446	7.08931858463641
H 35.23904337209275	-23.74008342773182	11.52081790009361
H 39.76178843720057	-23.15972843331156	4.26240638557155
H 38.67248600584563	-21.82532476438069	4.67976107481102
H 39.26591231322731	-22.91289287755783	5.94183605908716
H 35.50568127089106	-31.62528832348926	4.58343179323804
H 34.55753090700264	-33.06403479044335	5.00602160902400
H 33.75064674356324	-31.63706438802599	4.33081843833500
H 33.38076117163982	-31.75291146958907	6.79742941436076
H 35.13978928846537	-31.77486487179334	7.07074118873843
H 32.14695138966172	-26.37756163484892	7.51097121012792
H 31.28991249453635	-27.60347762080041	6.54785663876375
H 31.96583364539814	-28.04782643423488	8.09732400773670
H 37.31568654634227	-23.49510475132124	2.65158557923619
H 37.26233941170994	-24.75418604893386	6.65847421611496
H 35.39182457980549	-25.15207720117836	2.93599221495099
H 32.24117221127405	-26.83778375920444	2.00432000916548
H 36.80189888167848	-26.72890536915470	9.73912468796353
H 37.57938700041008	-29.61381885700174	4.11516287786563

H 32.36722203276216 -22.99473831256794 7.08832492150897

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B3LYP Scan/Melmid IPC Model/RKS/50 degrees Constrained Optimization

C	38.92464617452321	-22.86630705786361	4.90521041422723
C	37.74472774861374	-23.76587302520021	4.73221877379491
C	37.07131732529866	-24.58312107810847	5.60463768977725
N	37.08091072130654	-23.92707250933692	3.52402972030926
C	36.06312506846345	-24.81199321541107	3.71386177967168
N	36.03418748760809	-25.22465537680808	4.96153500181705
C	30.56902966228870	-24.69540060855688	2.40041339292779
C	35.63758995915032	-24.59926770271347	10.95279531276955
C	39.14726071674458	-30.00229601487648	6.26935000597735
C	33.63519019300244	-28.71718800465078	0.63330257548403
N	33.14881275899771	-25.53595762016520	5.00019294162024
N	34.58867102150609	-25.52154500563686	7.46474723257671
N	34.78137705152189	-27.68395286031476	4.05941632437217
C	32.84236492558527	-26.74586391549080	2.89245146792730
C	32.89433794270634	-23.88758561487060	6.79199031160995
C	36.30408385410669	-26.68790016892098	8.76269822478323
C	36.83599248511277	-28.92815594422152	4.51572138855504
C	30.67112564898451	-22.71370343866237	4.98283275135072
C	33.41977215242385	-22.64654147367336	9.58414948804482
C	38.70890425803182	-28.59585531290312	9.17326173523514
C	36.40766402010351	-30.07413464358637	1.66011661443656
C	32.50586154737874	-25.75372554162496	3.81013605588749
C	33.82244147366681	-24.40893602268244	7.68865441536963
C	36.75373440081869	-27.55683331219783	7.77291178406185
C	35.76635740313810	-28.56421094588132	3.70290546138888
C	31.46883585244429	-24.75368128207057	3.59960606347075
C	34.07951348217934	-23.86878360452804	9.01650409214515
C	37.90796928773827	-28.43396314259817	7.91509054718686
C	35.52391447332653	-29.08876637523691	2.36688588216458
C	31.51249624120286	-23.91929616562933	4.68424844496900
C	35.01019690258855	-24.69065057752709	9.59311448669676
C	38.09260397247123	-29.02452255129966	6.69506175819370
C	34.35916958326375	-28.51377024727333	1.93133153001428
C	32.56299487538580	-24.43011504367096	5.55321770162591
C	35.32499999428950	-25.71073171447111	8.60277439910204
C	37.03231433779898	-28.52256939993338	5.83143740419206
C	33.92147242986906	-27.62041958150464	2.99356262231900
N	36.23938819439245	-27.63886291351939	6.50764069009790
Fe	34.60749263136002	-26.68309917033127	5.81089594279613
C	34.28419997589736	-31.45080031075518	6.47060868521739
C	34.72294749224439	-31.97761271701266	5.11452573115177
C	32.15332681948617	-27.45350726256706	7.19548572130723
C	33.40223305968972	-27.83696657676592	6.45727681288774
C	33.33363235442329	-29.30034114374095	6.11973908474624
O	32.36855478231670	-29.80441000631683	5.58488102550433
O	34.38816055288278	-30.00964490286223	6.56574692134112
H	29.94983580064775	-22.51733273220978	4.18324948824736
H	31.28262204517468	-21.80911437318634	5.10180834556239
H	30.10052894577122	-22.83788486342337	5.91306195711028
H	31.13829660654941	-24.58038888600720	1.46797424210214
H	29.96995014749052	-25.61014915033475	2.29785722229378
H	29.87191481325542	-23.85394833140468	2.46206690303649
H	33.45874875326369	-27.76765463129383	0.11063741010581
H	34.20160244150032	-29.36252751910390	-0.04549507851865
H	32.65341112022886	-29.18444363816783	0.78766652497586
H	36.07096427121304	-30.24958033882685	0.63349943416651
H	37.44733944517532	-29.72432343073694	1.60891110326498
H	36.42233234931152	-31.04769866673024	2.16863659265187
H	33.79889981471958	-22.41504577379690	10.58447352954047
H	32.33167772203971	-22.77199004038744	9.66751522109138
H	33.59220496933134	-21.76330752491331	8.95449677082556
H	36.72837203407730	-24.48556085752916	10.89067225093056
H	35.44483890504473	-25.49980448112921	11.55122723795350
H	39.53830371460222	-29.29602656772360	9.03309170483835

H	39.13844462272703	-27.64240582197062	9.50984438446964
H	38.09405661472708	-28.97828200599965	9.99925636243405
H	38.71293039777150	-30.96414100350732	5.96451201480692
H	39.72565391411192	-29.62762402976191	5.41410094574680
H	39.85637526030008	-30.20792076940844	7.07760481453798
H	35.25122302890296	-23.74437483842557	11.51645174967547
H	39.76459051342169	-23.15555381850658	4.25918132891832
H	38.68270834373553	-21.81766674332721	4.68464517285707
H	39.27377707089965	-22.91337498525128	5.94079829608686
H	35.74432577859054	-31.66453375246914	4.89073137724641
H	34.68761768938752	-33.07224607182964	5.11482852655195
H	34.06502720653217	-31.61139083987642	4.32563221962918
H	33.25429275448420	-31.74189498983243	6.68613586754347
H	34.93578339655451	-31.81279464818811	7.26746725633319
H	32.13918502087718	-26.41352552371944	7.50528382726810
H	31.29847427071866	-27.64804601270025	6.53581394948552
H	32.00231137871179	-28.09307687916929	8.07693793403599
H	37.31066856413619	-23.46961821056291	2.65360369631153
H	37.26634763690880	-24.75171120368292	6.65335728351346
H	35.38185426073605	-25.12126502816963	2.93489707362878
H	32.24551074982222	-26.80199254228814	1.98757519158202
H	36.81106419327862	-26.72680871579636	9.72181924818670
H	37.55479583737549	-29.62893597738018	4.10231427657618
H	32.35005128455879	-23.00177877029773	7.10394363128974

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B3LYP Scan/Melmid IPC Model/RKS/60 degrees Constrained Optimization

C	38.92141728981282	-22.85452597894322	4.91554598804664
C	37.74322357487794	-23.75400670403261	4.73084705580177
C	37.06843081890413	-24.57990579614126	5.59399865030484
N	37.08258163753721	-23.90461488032695	3.51956358714408
C	36.06528946732208	-24.79238924987125	3.69845070326154
N	36.03379015490149	-25.21657188339429	4.94223975070806
C	30.58849257712114	-24.63400881021139	2.36860787766443
C	35.61974481096313	-24.65309512026587	10.94537508179813
C	39.13169181402511	-30.01801881108230	6.21405079767254
C	33.62644567669402	-28.66624420255229	0.58298419229440
N	33.14431364812826	-25.52094984802539	4.97680449117085
N	34.58513453203005	-25.52855300758510	7.44125502619560
N	34.77257692715788	-27.66621664037512	4.01899008704375
C	32.84733594135133	-26.70162241491416	2.85127679915642
C	32.88181719826186	-23.89583368712139	6.78892833594460
C	36.30289329530800	-26.70565062217001	8.72742968239362
C	36.80950909035334	-28.94096639942922	4.47441396382696
C	30.66964641843380	-22.69546644733021	4.98397218113905
C	33.39074534939242	-22.69548920021230	9.60187510656126
C	38.70679682933458	-28.61778943058776	9.12259392674959
C	36.37036137149091	-30.07436632042010	1.61775752714566
C	32.50980084794199	-25.71945428918205	3.77894000656531
C	33.81118543080445	-24.42475246002259	7.68010108497412
C	36.75016837224538	-27.56925695115194	7.73174607047209
C	35.74546572725737	-28.55991045126586	3.66205121756989
C	31.47690190484779	-24.71371140200905	3.57500466972537
C	34.06186267392720	-23.90289802732151	9.01637267856622
C	37.90145145650688	-28.45081972263018	7.86795559511705
C	35.49997113352202	-29.07639777825785	2.32347181122240
C	31.51247031935155	-23.89693956394972	4.67310215800957
C	34.99752419831652	-24.72658877332670	9.58231694715759
C	38.07829624118846	-29.04155181807491	6.64675532040101
C	34.34715759588506	-28.48059595530260	1.88531859561482
C	32.55628564156950	-24.42207052160384	5.54165134115660
C	35.32078666458202	-25.72987369501176	8.57790997538752
C	37.01580294851851	-28.53517122274346	5.78873518002760
C	33.91759279542909	-27.58698913627960	2.95082142350496
N	36.23127166945086	-27.64617682849156	6.46798433277243
Fe	34.60289588994610	-26.67536372056908	5.77683070091621
C	34.25326957603399	-31.44687450373144	6.66864206659556
C	34.86345628479005	-32.00005400930154	5.39198694569275

C	32.16415956663642	-27.47009342930137	7.18888911604870
C	33.40860833617206	-27.83472410193926	6.43326861847338
C	33.37323519775143	-29.30333888212867	6.13269704049281
O	32.49081496865514	-29.81172725576860	5.47490826858203
O	34.34661136419880	-30.00300170871155	6.74741061022217
H	29.95265834817107	-22.48798602357677	4.18331472147860
H	31.28031830401927	-21.79257463389667	5.11903823870441
H	30.09395611869526	-22.83284108052515	5.90921178800746
H	31.16705715341930	-24.50709975343160	1.44345280959027
H	29.98710796242473	-25.54485409054691	2.24650379212289
H	29.89397706314016	-23.79088367778323	2.43640541369536
H	33.46779751728052	-27.71140618847735	0.06417899670494
H	34.18616048356028	-29.31681898536749	-0.09635288213821
H	32.63670560093543	-29.11870661441150	0.73024378967828
H	36.02996176442722	-30.24827094534159	0.59209232041487
H	37.41429376667118	-29.73761874857040	1.56381081615543
H	36.37395575308889	-31.04646446015549	2.12927813892306
H	33.76527430213532	-22.47716410022354	10.60687944668791
H	32.30350171288023	-22.83127776001205	9.68009186516663
H	33.55747486861349	-21.80069441109277	8.98718298249742
H	36.71018153242665	-24.53341431980184	10.88893343161852
H	35.42914309597798	-25.56385349820082	11.52888134159285
H	39.53571250997654	-29.31736963443421	8.97670344137124
H	39.13720764951591	-27.66580898542607	9.46200205863313
H	38.09455161147065	-29.00399744331370	9.94879925856889
H	38.69862250217927	-30.98028759540652	5.90869315034704
H	39.70549243694942	-29.64023054752800	5.35709556465103
H	39.84477402747920	-30.22449262563224	7.01857464126309
H	35.22734983479815	-23.80892373151159	11.52090699431657
H	39.76379498915986	-23.13689984989128	4.26963803679882
H	38.67882535781717	-21.80425583326265	4.70365149769145
H	39.26729400602012	-22.91045251595783	5.95179027269044
H	35.90366045980875	-31.68492995214947	5.29128544205459
H	34.83248142160529	-33.09462012316975	5.41199495653088
H	34.30903521194110	-31.65480548929862	4.51857881031741
H	33.20343123733949	-31.73418461965593	6.75442752718985
H	34.79441065681928	-31.79151354249192	7.55110023761048
H	32.12178412477758	-26.42262524277573	7.46989072050836
H	31.30015899122922	-27.70990406749159	6.55572725656535
H	32.05869589197805	-28.08957229302882	8.09123631882729
H	37.31415960790115	-23.43894673490605	2.65399142812577
H	37.26020928363521	-24.75750273643269	6.64179391991766
H	35.38697268276362	-25.09606553502894	2.91472026313090
H	32.25583175229701	-26.74377035542302	1.94210890026137
H	36.81050446492961	-26.75228122312100	9.68584925274599
H	37.51777234409177	-29.65178768493259	4.06002688858465
H	32.33327335171969	-23.01655677624579	7.11169726310485

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B3LYP Scan/Melmid IPC Model/RKS/70 degrees Constrained Optimization

C	38.91945540789664	-22.84171816266160	4.90837362235446
C	37.74686658834829	-23.74821322492615	4.72227541798518
C	37.07628513823649	-24.57872831826467	5.58421143775011
N	37.08729340000075	-23.90061733735830	3.51066043177453
C	36.07420516481181	-24.79325589189184	3.68805937655468
N	36.04438632941486	-25.21924424182762	4.93144926675635
C	30.59631710311243	-24.62239238422307	2.35676464536799
C	35.65718056860033	-24.62549254548040	10.91858200757713
C	39.10057967989023	-30.06448450689610	6.22072895482238
C	33.62790108110506	-28.66044792542366	0.56987261724378
N	33.15747892761288	-25.50736392528266	4.96005817425628
N	34.59575695981091	-25.52071811606241	7.42699565995440
N	34.77950857648779	-27.65947231430878	4.00334189649827
C	32.86386347372269	-26.68211758019389	2.83099000382093
C	32.89112293720526	-23.88831481324662	6.77718080460895
C	36.31849250575321	-26.69464004418584	8.71013046379361
C	36.78949982927036	-28.97151170811778	4.47449150071239
C	30.66854338679059	-22.69462625238357	4.98045479963989

C	33.41695831433277	-22.67637887897427	9.58175066759317
C	38.70762422242426	-28.62251621470723	9.11307813125239
C	36.34527035333340	-30.10658416885071	1.61969274820323
C	32.52416588869425	-25.70339375028224	3.76119764423176
C	33.82439220432855	-24.41510812219912	7.66558799258884
C	36.75461288753682	-27.57032339261045	7.72005874001285
C	35.73745950529118	-28.57278961893336	3.65525752363101
C	31.48688028367697	-24.70127275116899	3.56155654274700
C	34.08391477942106	-23.88684856618091	8.99765396380044
C	37.89695737008824	-28.46248763655056	7.86089717625755
C	35.48914330782095	-29.09084022943533	2.31771486573635
C	31.51839359849200	-23.88944516143113	4.66333987861019
C	35.02382646529469	-24.70737356739210	9.56104187882296
C	38.06063815474829	-29.07058407386983	6.64630362024082
C	34.34845670030165	-28.47777066460099	1.87256200647365
C	32.56526630884070	-24.41315502947345	5.52937477276357
C	35.33879464224962	-25.71674482880548	8.55995179909942
C	37.00122585827589	-28.56059573736642	5.78655689923845
C	33.92862295801989	-27.57371406831878	2.93311450348165
N	36.22977564456649	-27.65477882959970	6.45893068625861
Fe	34.61226755167838	-26.66704717656910	5.75948450874016
C	34.10000970293069	-31.45815102751319	6.72194337984970
C	34.90726466023079	-32.01765990422553	5.56340265592075
C	32.18487463903196	-27.46878070069727	7.19924165299555
C	33.40955819489893	-27.82245808829837	6.40805422894356
C	33.36639191656875	-29.28419517681176	6.08538361518314
O	32.57322936527743	-29.75463678207670	5.30000942354062
O	34.21845614416422	-30.01784584354824	6.82976727498714
H	29.94816604023320	-22.48924569965314	4.18228564743439
H	31.27334912908273	-21.78800976226673	5.11716002408381
H	30.09605476749198	-22.83901605434262	5.90663209828313
H	31.17278226279871	-24.49118131054565	1.43091257482996
H	29.99862802384140	-25.53557312541109	2.23374740086352
H	29.89838186355244	-23.78233285054270	2.42756682940857
H	33.47293849884370	-27.70518581653627	0.05085656103804
H	34.18534649224449	-29.31341124416708	-0.10906651202667
H	32.63652729277177	-29.10939493501435	0.71727363482608
H	36.01224096760279	-30.27137222619731	0.59010766231159
H	37.39678344236700	-29.79261426890344	1.57762146184490
H	36.3223883394363	-31.07966367792592	2.12895110336303
H	33.79897882354504	-22.45265868072838	10.58276445700366
H	32.33033323784495	-22.81192805116932	9.66891750850886
H	33.57875945090667	-21.78479408735429	8.96110954437074
H	36.74727661776384	-24.50752852160821	10.85239962097094
H	35.47046590555002	-25.53184787713139	11.51016616494636
H	39.531443304015144	-29.32862055114708	8.96972952030112
H	39.14594699310793	-27.66998300232439	9.44066534997526
H	38.09753721251259	-28.99669587250698	9.94639124118789
H	38.65454691340601	-31.02373103922507	5.92453969363184
H	39.67811790885040	-29.70234683318889	5.35950086227219
H	39.81210453653980	-30.27291160219430	7.02614969950694
H	35.27058066870369	-23.77679521804758	11.49142171434765
H	39.76243080630532	-23.11574567513871	4.25966785503166
H	38.66918164506517	-21.79230463329462	4.70103833046936
H	39.26773810632888	-22.89922768987237	5.94371608845934
H	35.95766517397456	-31.73224361370362	5.64892292548577
H	34.84371575604764	-33.11087735929591	5.56272117176645
H	34.52290147852008	-31.64804159340466	4.61186520425645
H	33.04369558356644	-31.71533348038528	6.62290182026848
H	34.47068927926688	-31.82457930829267	7.68051508008243
H	32.11531831772971	-26.41220824765105	7.43817152153668
H	31.29622660974886	-27.77275109663704	6.63083466158199
H	32.16194715737942	-28.04715212455670	8.13490812771553
H	37.31656263330161	-23.43264448041371	2.64573103842989
H	37.26885835910983	-24.75667006153100	6.63177106190344
H	35.39700014881585	-25.09863196160549	2.90410860400647
H	32.27358686715990	-26.72178590286105	1.92092449522349
H	36.83150741213828	-26.73600266483728	9.66594065642978

H	37.48494404886185	-29.69851946989750	4.06674707685939
H	32.34200049294384	-23.00993513826260	7.10144425453375

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B3LYP Scan/Melmid IPC Model/RKS/80 degrees Constrained Optimization

C	38.93608493825806	-22.86796381358105	4.97296708812698
C	37.75525196152695	-23.75614376318697	4.75374001420025
C	37.06791563286737	-24.60046222441594	5.58865840661258
N	37.10534275946472	-23.87121957780585	3.53279211868398
C	36.08116134349910	-24.75684750094982	3.67869552147527
N	36.03545804939910	-25.21320026091335	4.91080317976628
C	30.64578512748494	-24.47158409398515	2.28841993574867
C	35.57538398777606	-24.79879171074355	10.92022542917014
C	39.06761594289031	-30.08713040779688	6.08007938213157
C	33.61121960337744	-28.53361794587160	0.45035451378773
N	33.14636804606926	-25.47650729523262	4.90759156949991
N	34.56175153829516	-25.56870907339933	7.38531514511166
N	34.76140303022279	-27.61289082243187	3.90689588097915
C	32.86857323710797	-26.58422591371086	2.74126730745623
C	32.86938785441445	-23.91047573807734	6.76895585881392
C	36.27085774561333	-26.78619276879635	8.64799091473665
C	36.74145492619583	-28.97405394610072	4.36508189475367
C	30.69891462080553	-22.62685666421647	4.97150521413412
C	33.35092507559013	-22.80553353595914	9.62416508246325
C	38.66530835233390	-28.71706003217208	9.00836811792586
C	36.28175337004845	-30.06403807661129	1.49845165928218
C	32.53047872913339	-25.62608405127749	3.69365079200034
C	33.78607896101371	-24.47343369578869	7.65295697041114
C	36.71158890916265	-27.63701173356505	7.63816635961274
C	35.70014624624613	-28.54197876765606	3.55003917390347
C	31.51182857116655	-24.60231109811525	3.50637435496190
C	34.02792190052195	-23.99303206281546	9.00582601196144
C	37.85307278495292	-28.53270881214020	7.76051469572379
C	35.44851880324214	-29.03462883779478	2.20330960673045
C	31.53600696237901	-23.82481941997349	4.63271260048731
C	34.96237272331031	-24.83166693754437	9.55145822765332
C	38.01841355977407	-29.11432319372538	6.53222832935761
C	34.32654979074652	-28.38857454491460	1.76048618130578
C	32.56059713558300	-24.39005657067058	5.49930247945427
C	35.29175591858417	-25.80470796608383	8.51992606244077
C	36.95839112557492	-28.58670820048339	5.68408292774590
C	33.91850411026132	-27.49375963427006	2.83399725737208
N	36.18908960977144	-27.69267814439789	6.37447193023831
Fe	34.58691375679135	-26.66830032790957	5.68801759083869
C	34.13832153391972	-31.37586254541743	7.14955464748329
C	35.28228191201040	-31.95011722903442	6.33324135961445
C	32.08835741445842	-27.50378467623755	6.98495216653010
C	33.38830601926313	-27.83878466940269	6.31526236638821
C	33.47124550988314	-29.32175103051437	6.13650619626171
O	32.91116633116946	-29.91078995246168	5.24022674279336
O	34.14439609737037	-29.92656745184446	7.13903763325537
H	29.98593222122453	-22.39514135978676	4.17391418260217
H	31.31387626092252	-21.73092629357281	5.13183392979167
H	30.11921072249947	-22.78485258814683	5.89088732685850
H	31.24174090937732	-24.31505992657879	1.37893387930113
H	30.04062210076337	-25.37290332635378	2.12192227740065
H	29.95591499272369	-23.62639578631824	2.37522669500205
H	33.48760488999350	-27.56766514629741	-0.05738353558377
H	34.15530854769010	-29.19332748437381	-0.23279641679742
H	32.60634256300859	-28.95620461692758	0.58399024402036
H	35.95491274911306	-30.20373006508283	0.46316501161603
H	37.34261975658084	-29.78149298409013	1.47154436522927
H	36.22347328061264	-31.04313380280398	1.99312514544412
H	33.71708330869964	-22.61865579537682	10.63856409404179
H	32.26324007165018	-22.94472859279539	9.68932593963430
H	33.52135638332715	-21.89127278107725	9.03979812443804
H	36.66721575214563	-24.68776251302470	10.87426928679274
H	35.37254812613576	-25.72233018632245	11.47906916159784

H	39.48292949471001	-29.42798055137300	8.85359435391467
H	39.11210093171172	-27.77281672565057	9.34822969572364
H	38.05359074711027	-29.09750809678608	9.83752260205729
H	38.63000897952745	-31.03779361984771	5.74697527166039
H	39.64778985933093	-29.68995788943084	5.23625536127242
H	39.77517578470666	-30.31871517397409	6.88266067930932
H	35.18678191712159	-23.96579943526035	11.51440848863156
H	39.78342121709171	-23.13810835503550	4.32829675584307
H	38.70065637145132	-21.81142294750945	4.78548729561531
H	39.27126119304911	-22.95184283278799	6.01082464737395
H	36.23932078874896	-31.55984343763575	6.68562822325069
H	35.29419787460062	-33.04139872045521	6.42423532475722
H	35.17015935906694	-31.69213407914119	5.27895135235122
H	33.17368286871222	-31.72523929374290	6.77801398053688
H	34.23227305412197	-31.63368349434964	8.20595255078669
H	31.95229682511037	-26.44021019147270	7.15643647320164
H	31.26399711120852	-27.87359691846966	6.35944697592181
H	32.00810743316725	-28.03625320885557	7.94356556163429
H	37.34775439474258	-23.38478878573183	2.68174780000186
H	37.24838156809636	-24.80696535181066	6.63311195924835
H	35.40872535977757	-25.03637976586087	2.88115958283941
H	32.28910903505297	-26.59216493077005	1.82337902267395
H	36.77679735383298	-26.85500984730868	9.60596006551318
H	37.42552437240407	-29.70572757098022	3.94685756801555
H	32.32154889454671	-23.03946489983270	7.11454549709030

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B3LYP Scan/Melmid IPC Model/RKS/90 degrees Constrained Optimization

C	38.95219118934335	-22.87796101003985	5.01111201712182
C	37.76575962407201	-23.75442783181949	4.77576897679178
C	37.06762117681146	-24.60255378338105	5.59766535039324
N	37.12228415318991	-23.85199662339006	3.54983471957459
C	36.09110130852602	-24.73180297102817	3.68039860775294
N	36.03507615088259	-25.20092031612170	4.90727831971614
C	30.65764120003080	-24.43091599095910	2.26359673495409
C	35.54303371892766	-24.85355770283357	10.91643666084918
C	39.03467134483105	-30.12166600174661	6.04759546251623
C	33.63278771931935	-28.47300462603287	0.39658099314713
N	33.14327082916558	-25.46722343352343	4.88490071973828
N	34.54744904811710	-25.58561157027718	7.36821310276385
N	34.77038115235480	-27.58462448653889	3.86576050010543
C	32.88248732834162	-26.54496318912171	2.70183295264847
C	32.85153274214251	-23.92605040245226	6.76484372743333
C	36.25313509337758	-26.81413466965266	8.62520966120430
C	36.73567597588992	-28.96660166670482	4.32504155883356
C	30.68899889992501	-22.62362616014049	4.97210345079028
C	33.31793207565132	-22.85268388761595	9.63380045905422
C	38.63759201784806	-28.75815110097016	8.98087386202080
C	36.28685530975080	-30.02863765840689	1.44771163395861
C	32.53582240608150	-25.60064713235811	3.66497558782204
C	33.76655736324846	-24.49649366936048	7.64568396420445
C	36.69588469974212	-27.65749636450966	7.61012737167524
C	35.70472558548474	-28.51685074659915	3.50689887063898
C	31.51576631580477	-24.57701945173411	3.48535956497636
C	34.00129560208929	-24.03093526502832	9.00480324110301
C	37.83151587350086	-28.56071459402405	7.73087446912718
C	35.45819968026671	-28.99720818366968	2.15472942040832
C	31.53056999822869	-23.81538499037384	4.62266019420614
C	34.93670525452870	-24.87240125232543	9.54443842620377
C	37.99740504989629	-29.13645889263054	6.49960493814186
C	34.34264901851842	-28.34150120025701	1.71105335057926
C	32.55103702120037	-24.39011820732389	5.48767784120895
C	35.27353195708940	-25.83232957191866	8.50321259124679
C	36.94610993285050	-28.59489186835186	5.64978505749917
C	33.93296613061198	-27.45397026132505	2.79011229277048
N	36.17874437379107	-27.70129988186996	6.34336266125815
Fe	34.58276015741146	-26.66540731328188	5.65675185502804
C	34.10622233977196	-31.35181881233827	7.25920337094367

C	35.36781424406704	-31.89349304984197	6.61001981172507
C	32.08909245727730	-27.53803667369267	6.94355825551785
C	33.39262037757496	-27.84972914844460	6.27076363179452
C	33.53009914735660	-29.33239132219649	6.12300227555608
O	33.14021664066148	-29.95038438068847	5.15971303859522
O	34.05943594546324	-29.90367826004689	7.22816964161106
H	29.97659368307493	-22.38638664363710	4.17561886889558
H	31.30078164747061	-21.72725345273289	5.14212789813223
H	30.10832286725291	-22.79240251967135	5.88892485821794
H	31.25928884576244	-24.25887094637550	1.36067450416884
H	30.05648360511782	-25.33148483817240	2.07941217361255
H	29.96448790729037	-23.58926866537421	2.35831074954621
H	33.51500466087863	-27.50249044267720	-0.10379189719430
H	34.17742952082347	-29.12931273438484	-0.28938374091355
H	32.62572174656416	-28.89304162357217	0.52202703700819
H	35.97365366555451	-30.14869613763835	0.40573323386612
H	37.35198340620938	-29.76175667744745	1.44052752464006
H	36.20603404005061	-31.01354631608580	1.92740523560754
H	33.67792577315638	-22.67708041283821	10.65241475868843
H	32.23026222701185	-22.99524731405169	9.69124041915861
H	33.48931463301508	-21.93096618169639	9.06153337511842
H	36.63530699749259	-24.74471917472556	10.87698740902873
H	35.33515840399131	-25.78163264786718	11.46589234654698
H	39.45037060674264	-29.47443829912817	8.82529240601161
H	39.09025836900278	-27.81916570779850	9.32743402827820
H	38.02004037460455	-29.13830801296006	9.80580940437672
H	38.58402314362128	-31.06957277428840	5.72372660222385
H	39.61400310672953	-29.73611964130972	5.19799132269762
H	39.74428508240585	-30.35558900189156	6.84772069849002
H	35.15343479641862	-24.02506675216220	11.51625919641841
H	39.80201859487281	-23.15005096724781	4.37053769629894
H	38.72703469981838	-21.81798938500048	4.83064597976148
H	39.27886797359015	-22.97322142808293	6.05069412650205
H	36.25638846869267	-31.46396859283017	7.07681908425899
H	35.40516361390802	-32.98231044029549	6.72166054377499
H	35.38664015978613	-31.65424901740828	5.54595603808756
H	33.21166250507529	-31.74130576976065	6.76999843215697
H	34.06955062993430	-31.59466893417511	8.32253715929663
H	31.92545787746062	-26.47524647389901	7.09539053018562
H	31.26520481137985	-27.94085932085706	6.33688044517672
H	32.03736027247243	-28.05406101031461	7.91244912072629
H	37.37336499639829	-23.35866604003676	2.70531372090985
H	37.24039400108632	-24.82171138527973	6.64082798450171
H	35.42189087265699	-24.99889114469888	2.87592414368346
H	32.30835061410920	-26.54274356777417	1.78055154586846
H	36.75502050029827	-26.89232838473575	9.58458324601601
H	37.41593021014906	-29.70053931165595	3.90463703277640
H	32.29912144205255	-23.06133242351222	7.11886726218284

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B3LYP Scan/Melmid IPC Model/RKS/100 degrees Constrained Optimization

C	38.94404472945526	-22.86630614138057	5.03892014724524
C	37.76268825773936	-23.74607857390899	4.79070298163154
C	37.06680134052296	-24.60708009041944	5.60111328881300
N	37.12162336851922	-23.83165774715440	3.56257737210432
C	36.09422514642817	-24.71760013129965	3.68080557734271
N	36.03799902064166	-25.20151299232264	4.90191338999397
C	30.66039483433126	-24.42257296617673	2.24918389008752
C	35.52815353678274	-24.89665389853475	10.90947985221320
C	39.02564173711591	-30.14135596890430	6.01934448230701
C	33.67383633832022	-28.41955457108606	0.34670659361621
N	33.14476876276408	-25.47014231169043	4.86683794037960
N	34.54278452796316	-25.60450146134605	7.35370096180433
N	34.77912318158284	-27.57559532782811	3.83764969824831
C	32.89569488195210	-26.52854787522962	2.67326249302113
C	32.84608060093529	-23.94314267638304	6.75744795402003
C	36.24451711163866	-26.84163789627554	8.60805130468857
C	36.74104892301729	-28.96362230471756	4.29459924812938

C	30.67838249578458	-22.63792784056812	4.97289558159443
C	33.30493581586471	-22.88840642590202	9.63470673973780
C	38.63183493002767	-28.78454198240343	8.95645455943426
C	36.32182099691039	-29.98392011686924	1.40061166597116
C	32.54092786281761	-25.59549374747622	3.64431466490617
C	33.76075838402266	-24.51762396370947	7.63619759379043
C	36.68839882677445	-27.68072377695121	7.58995208290245
C	35.71745259149441	-28.50202592041506	3.47459062357411
C	31.51690403565717	-24.57477028429321	3.47132472794313
C	33.99152686986678	-24.06115388573274	8.99905225556715
C	37.82450746261848	-28.58378542665085	7.70764592808303
C	35.48347653179063	-28.96500607818850	2.11420500429249
C	31.52649548620301	-23.82239440484513	4.61482760150336
C	34.92582425117106	-24.90581819365461	9.53563329640080
C	37.99181787515369	-29.15399353944864	6.47387218938609
C	34.37010779213251	-28.30637134123318	1.67009936104116
C	32.54806856571903	-24.39965856011361	5.47693267087334
C	35.26570210764663	-25.85878349288305	8.48918347998005
C	36.94270737375813	-28.60786108999293	5.62482382933812
C	33.94949914915448	-27.43411058464712	2.75762766019777
N	36.17238741281793	-27.71934519144965	6.32228597985752
Fe	34.58056501580486	-26.67475046206500	5.63453500041907
C	34.03096556855976	-31.34124745995868	7.34110090984085
C	35.35750737880123	-31.84480116493299	6.79864704925500
C	32.10474133160970	-27.54106306389037	6.95505305625194
C	33.38976830945600	-27.85715290739421	6.24994075973643
C	33.54589143149546	-29.34136863973454	6.12959905110940
O	33.30020735207680	-29.97604187969542	5.13110785387543
O	33.93727747384006	-29.89557868915730	7.30177678879064
H	29.96741521732447	-22.39653483189337	4.17638675002300
H	31.28534174050124	-21.74033020766186	5.15330061867690
H	30.09563365418936	-22.81818201964015	5.88623426268330
H	31.26239024721955	-24.23170242319300	1.350220622944007
H	30.07035939660808	-25.32759348055596	2.05158607990105
H	29.95713921415941	-23.59043550218598	2.35291855625663
H	33.56791651580225	-27.44301421171191	-0.14464926114028
H	34.22205599905939	-29.07203049499866	-0.34005731765546
H	32.66275723112392	-28.83443653198390	0.45596239946392
H	36.01871599280540	-30.09071643153144	0.35421039393385
H	37.38605038320683	-29.71348353653391	1.40679949422849
H	36.23969194434967	-30.97523602647864	1.86654953085253
H	33.66411460189089	-22.71793024152552	10.65447083658044
H	32.21762935171056	-23.03430783101600	9.69092642746964
H	33.47403387990237	-21.96289758273776	9.06797571892902
H	36.62048037725649	-24.78693722304851	10.87383879107768
H	35.31935071391818	-25.82893726839381	11.45138796352162
H	39.44597708688902	-29.49847125720662	8.79720209412501
H	39.08305171940975	-27.84584281338541	9.30566108017142
H	38.01643178047806	-29.16890658753530	9.78101170270259
H	38.57117748753537	-31.09076936557400	5.70518887156885
H	39.59778862073506	-29.76118821066558	5.16257934382438
H	39.74194589350328	-30.37069703825938	6.81480196433161
H	35.13639929560693	-24.07290246119101	11.51438169919149
H	39.79622078502985	-23.12517603832998	4.39599833949999
H	38.71304037270598	-21.80536945582073	4.87192657884742
H	39.26986682915278	-22.97307818138822	6.07763976308163
H	36.19297958929060	-31.37603309950662	7.32278397544848
H	35.42487616094632	-32.92971189242390	6.93223063948249
H	35.44874950868397	-31.62108519457805	5.73521994756982
H	33.19215705919895	-31.76084447209563	6.78267867147200
H	33.91495018026558	-31.58326831025983	8.39881277184691
H	31.92767965222365	-26.47630820703326	7.07267169207692
H	31.26198349812041	-27.98075641745470	6.40148290504801
H	32.10531706713606	-28.02000428415917	7.94352399457412
H	37.37136950238857	-23.32646313879020	2.72469986016313
H	37.23889697859008	-24.83804559335514	6.64182595152365
H	35.42676123512880	-24.97674224980831	2.87228846434913
H	32.32639379945647	-26.51907820521572	1.74901622552055

H	36.74490119390482	-26.92465605795567	9.56779376460534
H	37.42372431128092	-29.69285254326738	3.86999095013355
H	32.29121393756962	-23.08209612373517	7.11649543329934

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B3LYP Scan/Melmid IPC Model/RKS/110 degrees Constrained Optimization

C	38.94392888532710	-22.85391290398428	5.06186417389854
C	37.76303421504652	-23.73146394698377	4.80366713544504
C	37.07274068726389	-24.60890331829481	5.60122003010986
N	37.11594219741713	-23.79511668902757	3.57733977555857
C	36.09071960339958	-24.68498545513887	3.68414482148726
N	36.04138809681246	-25.19186175817375	4.89615259590428
C	30.66127826766117	-24.40839869828969	2.23718174860653
C	35.51818130507674	-24.94520894480232	10.89891918484093
C	39.03045796084596	-30.14617303877990	5.97449310636330
C	33.69641378097642	-28.37455609329787	0.30161751302297
N	33.14898164876148	-25.46914400997660	4.84648541782153
N	34.53767833805705	-25.62668710386872	7.33652237730750
N	34.79445159482171	-27.55497898794273	3.80054620148568
C	32.90739464278020	-26.50719018592880	2.64278865935054
C	32.84104859129121	-23.96139498779215	6.75127273576076
C	36.23869711030509	-26.87232583833262	8.58433181463374
C	36.75462038963700	-28.94806851705988	4.25078462005031
C	30.67065449930178	-22.64808199864557	4.97673121188522
C	33.29525525038776	-22.92902924179539	9.63674032259733
C	38.62899983127450	-28.81374929380889	8.92123892625378
C	36.34526301035593	-29.94295010235783	1.34966804830802
C	32.54692770011940	-25.58509655691073	3.62216080133449
C	33.75421191739462	-24.54277449734057	7.62668779409074
C	36.68634250914086	-27.70228509482762	7.56032910287076
C	35.73487518485488	-28.47672760565484	3.43221720697218
C	31.51861918715162	-24.56739965760307	3.45783969773987
C	33.98282968321097	-24.09690639125458	8.99319802437283
C	37.82423774768426	-28.60355604623254	7.67220430924052
C	35.50472854332150	-28.92923245686671	2.06773593928079
C	31.52421693877858	-23.82542945382804	4.60821761751487
C	34.91699670636490	-24.94510783715036	9.52451633437921
C	37.99509577060678	-29.16289112862446	6.43396171450737
C	34.39051018183434	-28.27028955571690	1.62687628107670
C	32.54713835549975	-24.40657079049918	5.46589447889711
C	35.25896640111905	-25.88961931060698	8.47123335457780
C	36.94837364847731	-28.61007771079743	5.58662233869358
C	33.96593766929698	-27.40772733188937	2.72066439893243
N	36.17277227119337	-27.73099461922392	6.29101412954241
Fe	34.58253708905792	-26.67981069610731	5.60698150945850
C	33.92060188604798	-31.34665809289499	7.39309396381285
C	35.34924820631170	-31.80053400286766	7.14817480397506
C	32.11051084633756	-27.56272434390163	6.91546732143064
C	33.39631365700714	-27.87213161953154	6.20896189788692
C	33.58840525654766	-29.35563142237581	6.11197656359818
O	33.52213980626242	-29.99897047543472	5.09209288377876
O	33.79485728806151	-29.90483715590656	7.33666776871802
H	29.96085857314815	-22.40093185167897	4.18095585520245
H	31.27373356664289	-21.75015850133773	5.16821382564250
H	30.08619428799075	-22.84015404300641	5.88658024957844
H	31.26245148384751	-24.21225972504809	1.33884264795745
H	30.07126831656070	-25.31245117500302	2.03496258381529
H	29.95785032099997	-23.57709651620906	2.34630067313846
H	33.59920789876873	-27.39595977989775	-0.18760919003542
H	34.24115541057095	-29.02953180980701	-0.38549509993691
H	32.68184087473444	-28.78180591531611	0.40731301583624
H	36.03905405368190	-30.04990284956079	0.30419490382494
H	37.40833388401010	-29.66776911738712	1.35266604820566
H	36.26869691399144	-30.93465373642002	1.81553670459240
H	33.65426801560563	-22.76502567376561	10.65763233728074
H	32.20805922356394	-23.07613654588850	9.69201101763868
H	33.46365941374165	-21.99960643778914	9.07626087992685
H	36.61077238881483	-24.83776882106003	10.86471835321308

H	35.30683539293568	-25.87993890922029	11.43561837801979
H	39.44447169292846	-29.52519105949907	8.75783233799208
H	39.07815291213255	-27.87738744085689	9.27930873696736
H	38.01257566771062	-29.20571172035403	9.74154694854739
H	38.57803392503143	-31.09498164716740	5.65566649244260
H	39.60177858246072	-29.76074204087601	5.11956024825404
H	39.74715566075139	-30.37812752974957	6.76877362619426
H	35.12793245530192	-24.12385495763836	11.50806405471720
H	39.79306163644585	-23.09900329282200	4.40955074208372
H	38.70977685203896	-21.79058549972050	4.91570871977128
H	39.27577116602861	-22.97908274840753	6.09660354887964
H	36.03583750204560	-31.32364017404556	7.85074569166205
H	35.42187848494418	-32.88626308977725	7.27204244679807
H	35.66462217197351	-31.54740672390496	6.13511383843897
H	33.23764720243522	-31.78570747732012	6.66406523114670
H	33.58567393630322	-31.60406642926990	8.39948175660893
H	31.87468790470432	-26.50307540897930	6.93422208192149
H	31.27339767575628	-28.10782394747246	6.45584353430876
H	32.18358827922007	-27.93166442470990	7.94744849368183
H	37.36073978971070	-23.27394582647965	2.74782972056545
H	37.25012627155901	-24.85904871323379	6.63661652045314
H	35.41984711481562	-24.93037117114927	2.87415909576898
H	32.33916978777463	-26.49225340996511	1.71793773566675
H	36.73750457531658	-26.96191829036398	9.54429694808120
H	37.43910339449965	-29.67218096316536	3.82046606998028
H	32.28351796501764	-23.10498572934630	7.11717523779278

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B3LYP Scan/Melmid IPC Model/RKS/120 degrees Constrained Optimization

C	38.93816056265536	-22.84436352054032	5.07522692479852
C	37.75879157344249	-23.72258757649006	4.81220676282219
C	37.07491751520134	-24.61189213897363	5.60226145863457
N	37.10596141887189	-23.77321753510887	3.58828001325868
C	36.08393994649421	-24.66755451193973	3.68927758185644
N	36.04195649132236	-25.18925382165571	4.89515261881514
C	30.65406329001579	-24.42035240233508	2.23490614583531
C	35.51197010582125	-24.96800534136893	10.89402093233771
C	39.04343175336849	-30.13821743874586	5.95437336522113
C	33.72695227355674	-28.34529247035352	0.27408061975627
N	33.14779599119377	-25.47877285107831	4.83921622682575
N	34.53492078412464	-25.64076143665957	7.32886708217899
N	34.80282972681458	-27.54952729454105	3.78540890689061
C	32.91071142424123	-26.50867383288242	2.63105364982914
C	32.84009799671588	-23.97306639220869	6.74593647486749
C	36.23138684382049	-26.89258992375673	8.57723526417677
C	36.77274205211103	-28.93096800117900	4.22968696698520
C	30.66283945496523	-22.66381968562184	4.97675707539318
C	33.29669110060001	-22.94353536195579	9.63176571039469
C	38.62427861227849	-28.83197794395378	8.91013846804735
C	36.38851991702080	-29.89595884288646	1.31708652193840
C	32.54501513361242	-25.59370873246196	3.61500748339837
C	33.75376372767100	-24.55544576775407	7.62014094794759
C	36.68284740345869	-27.71720540763545	7.55050458903294
C	35.75362380051224	-28.45820282752326	3.41189966230534
C	31.51337201325981	-24.57897380359666	3.45424384686812
C	33.98203171493821	-24.11222019094049	8.98734955101042
C	37.82343470652474	-28.61516916198223	7.65970219494802
C	35.53357841478569	-28.89938391168098	2.04207416216326
C	31.51858925209911	-23.83878197747668	4.60577393278881
C	34.91301042983219	-24.96405382193100	9.51864283238803
C	38.00174411576209	-29.16328232453536	6.41744527323631
C	34.41385005164700	-28.24838061339679	1.60364557561130
C	32.54415544438501	-24.41844468726838	5.46119523178142
C	35.25393715421533	-25.90755993770499	8.46424256516085
C	36.95659513405204	-28.60754672542819	5.57026263915256
C	33.97683457999553	-27.40066514608793	2.70427613808249
N	36.17352603840781	-27.73862044612124	6.27897353043626
Fe	34.57962885528813	-26.68973419663142	5.59693211121953

C	33.83366351566610	-31.36615483434977	7.39988035123719
C	35.28820714856771	-31.78147778625903	7.25671860802239
C	32.13986109546169	-27.56407970956723	6.95481167674461
C	33.39687897807396	-27.88331277648889	6.20230685757028
C	33.59716862567176	-29.36774282971619	6.10814935886718
O	33.66741881442347	-30.00631953187111	5.08589555170897
O	33.67228901233745	-29.92882396653153	7.34552708453087
H	29.94901295926655	-22.41978569947004	4.18364179777975
H	31.26389252678566	-21.76378303417357	5.16477417895185
H	30.08275079286050	-22.85676795494985	5.88917702330940
H	31.25340744182028	-24.21971406177429	1.33632665267505
H	30.06749567341376	-25.32631064117254	2.03124539544529
H	29.94746283396993	-23.59213663225934	2.34679286652704
H	33.62785125717188	-27.36336574446376	-0.20810017955698
H	34.27828610528558	-28.99240812423676	-0.41524186242369
H	32.71371466395784	-28.75799161387472	0.37111438970971
H	36.08742580637512	-29.99614927541176	0.26945984537839
H	37.44816100137374	-29.60801775090123	1.32689025935014
H	36.32214890868722	-30.89296317082149	1.77303542636036
H	33.65435337306144	-22.78232660009683	10.65357362799612
H	32.20900795703243	-23.08772918802017	9.68492913418937
H	33.46864525974960	-22.01360674564524	9.07321424844836
H	36.60512534678971	-24.86601957951322	10.86173166908901
H	35.29494234602086	-25.90192743281211	11.42986883311296
H	39.44167879115686	-29.54078824110962	8.74501666779826
H	39.07044996674129	-27.89703615067027	9.27563926931736
H	38.00594597625769	-29.23020175261988	9.72599449781994
H	38.59673173332235	-31.08627609210397	5.62560342098583
H	39.61675339158997	-29.74295729784875	5.10528739351996
H	39.75762550111568	-30.37361734021695	6.74986388696275
H	35.12487086332444	-24.14500211737468	11.50295183455662
H	39.78419793097413	-23.07747776843238	4.41453526627262
H	38.69940757069904	-21.77998948253439	4.94491970954828
H	39.27677040544827	-22.98234004225834	6.10613873045480
H	35.91066286522906	-31.28805449946682	8.00645137999666
H	35.38080889253308	-32.86500465121658	7.38563375083704
H	35.66705097609488	-31.51787463396108	6.26886069763528
H	33.21778725786647	-31.81710457063637	6.62007838423089
H	33.43308044186453	-31.64143268558907	8.37706838784607
H	31.89246966355764	-26.50700210773492	6.94702590857401
H	31.28595003193955	-28.13451674024307	6.56194839738300
H	32.26977499389988	-27.89293062312183	7.99431544763541
H	37.34539387860586	-23.24138326047025	2.76397468833126
H	37.25798613667761	-24.87424162919465	6.63366956799499
H	35.41026598614211	-24.90544910579369	2.87934601888005
H	32.34353908676920	-26.49162110480843	1.70560977039413
H	36.72763453776493	-26.98589060213859	9.53816392964196
H	37.46381417184134	-29.64626713881227	3.79526175594085
H	32.28249768467646	-23.11719376587005	7.11293110402316

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B3LYP Scan/Melmid IPC Model/RKS/130 degrees Constrained Optimization

C	38.93797881597923	-22.84788555190333	5.08569297548776
C	37.75558117122382	-23.71929827845092	4.81363710268141
C	37.08461633646787	-24.63402971500604	5.58555911770363
N	37.08420596817236	-23.73241037082633	3.59865143558441
C	36.06456919156214	-24.63080273440217	3.68732872166341
N	36.04131199048027	-25.19009990675948	4.87667123921771
C	30.65778801256490	-24.38980895924569	2.22395412600913
C	35.49096467324166	-25.08336117941930	10.88555232807406
C	39.08006766903859	-30.11854088783443	5.84487438178275
C	33.74781149230729	-28.27114107412019	0.20159498811970
N	33.14882824176834	-25.49081605838295	4.81351567823062
N	34.53619042820076	-25.68871302710441	7.30283880849295
N	34.80881245814670	-27.53779969196896	3.73136801019030
C	32.91128123475019	-26.48860841125629	2.59170659677587
C	32.83988221927557	-24.01412532259386	6.74269645363100
C	36.23391334492831	-26.95650894833059	8.53363064775241

C	36.79584746540024	-28.90334097219072	4.14746603888509
C	30.67209478813339	-22.67032640686913	4.98898665187404
C	33.27613206600721	-23.04158503327193	9.65059271859971
C	38.65038537063133	-28.87601809812409	8.82643119055974
C	36.42334477819515	-29.81574419214381	1.21837400469427
C	32.54536382386669	-25.58733831967076	3.58820735928680
C	33.74943495317337	-24.61217599743802	7.61052405016014
C	36.69268855953849	-27.75843388670538	7.49197418304239
C	35.77063547260977	-28.42765805195708	3.34042213971664
C	31.51594066532947	-24.56838051827976	3.44131261706408
C	33.96932047607893	-24.19490392145104	8.98711464302639
C	37.84423394867635	-28.64459759026454	7.58230831317525
C	35.55628602215188	-28.84375412007823	1.96207195495520
C	31.52394163067513	-23.84314759524796	4.60244679843407
C	34.90043027079987	-25.05385592748863	9.50688624044926
C	38.02644822894524	-29.16679247319729	6.3294252263251
C	34.42936525771503	-28.19704861842979	1.53544394943304
C	32.54768147652018	-24.43711405491976	5.44980930046836
C	35.25106964694790	-25.97493814908866	8.43636663510358
C	36.97402853859879	-28.60658065208173	5.49427781922325
C	33.98265171667556	-27.37520248193687	2.65178869424079
N	36.18131849151408	-27.76209269168919	6.22073715741570
Fe	34.5813131314806658	-26.71350267372256	5.55679832064984
C	33.74413828863270	-31.33395595200589	7.56033084226635
C	35.20523221841395	-31.62910499661454	7.85517285780075
C	32.10795015060582	-27.59234794515184	6.84246524679524
C	33.40323755796587	-27.91392714416206	6.15845605733164
C	33.66575205458849	-29.39476083191268	6.15447009958802
O	33.96884933981553	-30.06505326133762	5.19772291205077
O	33.51120742905169	-29.91567190865847	7.40642445671968
H	29.95835299513550	-22.41431859811905	4.19960741360117
H	31.27613425007632	-21.77451733849904	5.18739026250307
H	30.09236528542291	-22.87271359339605	5.89957692886931
H	31.25643953646889	-24.15683963090849	1.33258350064811
H	30.08436597440328	-25.29793057646977	1.99465822512553
H	29.93938749516079	-23.57473335013521	2.35568225982808
H	33.65334923220598	-27.28109338321594	-0.26482026017734
H	34.30109205145172	-28.90789505449841	-0.49574586552301
H	32.73306546736944	-28.68286095574042	0.28637422265328
H	36.12052453005634	-29.90338849176418	0.17011674800124
H	37.47866525658303	-29.51239544909480	1.22975758569203
H	36.37293859345107	-30.82051341887900	1.65886450955430
H	33.62618043193003	-22.90020221562309	10.67794742669941
H	32.18859339956631	-23.19006813149930	9.69327384097132
H	33.44909976336812	-22.09988835098223	9.11243086284942
H	36.58482404248912	-24.98745308140649	10.86122963440110
H	35.26516817695290	-26.02431858946652	11.40529384051927
H	39.47222053074449	-29.57618649407643	8.64711853734397
H	39.09112972259476	-27.94408154251015	9.20588072424232
H	38.03786247694968	-29.29231498625307	9.63757953869418
H	38.64289161062950	-31.05704703694683	5.47851742949325
H	39.65970726590455	-29.69034596495849	5.01616417414492
H	39.78700634370078	-30.37645975129332	6.63975374264091
H	35.10514674654157	-24.26778127457160	11.50520717415934
H	39.77416511566640	-23.05948397932559	4.40546393202218
H	38.69618163975790	-21.78038957914094	4.99152067626296
H	39.29234002979861	-23.01668309700342	6.10666872944260
H	35.54059732121749	-31.08054330189661	8.73865802691771
H	35.34271091696249	-32.69974036733562	8.03955400331346
H	35.83615062762163	-31.34125541724272	7.01293172396480
H	33.41236968616123	-31.84502102851043	6.65549716134072
H	33.10192152825771	-31.62436644457579	8.39395436867472
H	31.83627708690128	-26.54374967588853	6.77461083262274
H	31.28470857136301	-28.20186424391784	6.44345100430256
H	32.19931639592794	-27.86963661301541	7.90025185295717
H	37.31039016572090	-23.17433576889538	2.78806468635156
H	37.28346180683764	-24.92852605587401	6.60535026156343
H	35.37801592692247	-24.84289051895504	2.88100323945247

H	32.34458600462574	-26.45981011086735	1.66625817953732
H	36.72998300213846	-27.06351314519491	9.49321810532011
H	37.49400736097033	-29.60294395825431	3.69926383826264
H	32.28099853555860	-23.16493094310342	7.12301953371590

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B3LYP Scan/Melmid IPC Model/RKS/140 degrees Constrained Optimization

C	38.93018183287350	-22.81938043640480	5.09011552466699
C	37.75460393028734	-23.69832834660568	4.81286020077295
C	37.09130599969956	-24.62324807465250	5.57933047024466
N	37.08209434868045	-23.70849178952892	3.59846034312722
C	36.06929956391826	-24.61519445591650	3.68225933573824
N	36.05155197691757	-25.18220499206878	4.86794365150551
C	30.63390616163828	-24.43082310234209	2.23217605615830
C	35.47751584971337	-25.10653332627539	10.88374600953363
C	39.09470018424056	-30.11138127386353	5.83231978477167
C	33.76944476587467	-28.26628013635081	0.18786147705290
N	33.15785270807199	-25.49537115303380	4.80431011669716
N	34.54732114689867	-25.68826337904142	7.29087815941817
N	34.82440809597106	-27.53079050660555	3.71906111890748
C	32.91291511362628	-26.50190070721202	2.58671746425089
C	32.85004230934829	-24.01513021403166	6.73144234871374
C	36.23134471865026	-26.96995028545647	8.52776936937037
C	36.82890867048539	-28.87264255381052	4.12822889517181
C	30.65682279742422	-22.69706233802741	4.98877262423299
C	33.27826610548872	-23.05059994719470	9.64402589196344
C	38.63439440595248	-28.90877529120094	8.82632203696501
C	36.47351293039131	-29.76880266628321	1.19285806973815
C	32.54550578779806	-25.60239711622967	3.58417056353530
C	33.76103090312805	-24.61138594439501	7.59898637985927
C	36.69683801645701	-27.76530732683457	7.48418112280849
C	35.80006893670616	-28.40320267472873	3.32284884895529
C	31.50590141543928	-24.59341340122153	3.44195301814313
C	33.97424953666569	-24.20096113212706	8.97839542449017
C	37.84442546972098	-28.65684109176595	7.57588172231771
C	35.59069505049724	-28.81575548797242	1.94261826709732
C	31.51742325622903	-23.86255486608716	4.59963442179594
C	34.89875006488707	-25.06608789327066	9.50032612072231
C	38.03919952982280	-29.16241373133373	6.31814740220087
C	34.45213766525513	-28.18641701158382	1.52081278223412
C	32.55307545058302	-24.44386288603435	5.44142154154371
C	35.25385065877009	-25.98297916570295	8.42776832027904
C	36.99614515688143	-28.58986763742605	5.47930285489337
C	33.99478053823814	-27.37593360255346	2.64132174366853
N	36.19790530712815	-27.75360480734844	6.20807416673167
Fe	34.59218648547777	-26.71131116352925	5.54655749269820
C	33.65513224337025	-31.35481767913242	7.52666219311004
C	35.10072192984387	-31.63380857956026	7.90497432867015
C	32.16853788626722	-27.56347218804691	6.91731610939033
C	33.41977670472532	-27.91055329321813	6.16564416463317
C	33.68040559673427	-29.39172778104109	6.15374206949251
O	34.09043585423400	-30.04475315620610	5.22527437565084
O	33.40783715120146	-29.93945180483585	7.37543551229704
H	29.94464098321243	-22.44148925344008	4.19786173312306
H	31.25452730358266	-21.79873201527714	5.19429134590511
H	30.07455745856414	-22.90787340573771	5.89591203488136
H	31.22312424017188	-24.21836306854748	1.32960922337602
H	30.05205996398686	-25.33937931558829	2.02662138576657
H	29.92225541398528	-23.60893442523649	2.35773305886415
H	33.66676485770876	-27.27740415056607	-0.27935817217897
H	34.32659473250789	-28.89946347233976	-0.50967001498915
H	32.75803202031667	-28.68568022309422	0.27448057299875
H	36.16738138148013	-29.86107222708202	0.14598507179747
H	37.52245579455409	-29.44390124179339	1.19992323131172
H	36.44593259469749	-30.77505879978322	1.63200309643108
H	33.62606282684973	-22.91198381162366	10.67251165236992
H	32.19086290924391	-23.20096555745452	9.68414628938699
H	33.45079564832704	-22.10703567059604	9.10914520869052

H	36.57189219622622	-25.01487020032220	10.86956626897307
H	35.24344224094640	-26.05001704693780	11.39518285725553
H	39.46547288905819	-29.59712933261476	8.64391201810883
H	39.06034235318341	-27.98144742754680	9.23278674336253
H	38.01365849761336	-29.34871149895004	9.61859485815933
H	38.65880208737702	-31.04813299986547	5.46004014151150
H	39.67667621995233	-29.67888521961706	5.00755053340608
H	39.79937693754926	-30.37286598102501	6.62806492610371
H	35.08943066759407	-24.29363940836808	11.50548354500355
H	39.76750092834453	-23.01916072570162	4.40772650604772
H	38.67955476160454	-21.75325307218832	5.00393604944859
H	39.28669967963954	-22.99268486553735	6.10958084842134
H	35.37795282361349	-31.08381183441431	8.80785756004538
H	35.23862647277658	-32.70308452010576	8.09665850704285
H	35.77633192451913	-31.33813825174104	7.10127205054852
H	33.38575546629197	-31.86097079695687	6.59841367291876
H	32.96904278113313	-31.66457085838896	8.31719813411238
H	31.82582429085448	-26.55168065801267	6.72222696108749
H	31.3526565595933	-28.27040384693566	6.72282149182573
H	32.38981087860660	-27.64515701154930	7.98996469678361
H	37.30311576740682	-23.14315020590670	2.79149148277565
H	37.29330671300148	-24.92314305096302	6.59694934290505
H	35.38334234744410	-24.82705966496705	2.87533967401089
H	32.34050206563882	-26.47973108168355	1.66463404140617
H	36.71800231753286	-27.08587181274700	9.49114054795600
H	37.53540184603757	-29.56185020516966	3.67691765819978
H	32.28883693009146	-23.16754147853112	7.11184696862556

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B3LYP Scan/Melmid IPC Model/RKS/150 degrees Constrained Optimization

C	38.92478924539691	-22.78583785308534	5.06560962060234
C	37.74933178384065	-23.66741131514661	4.79621096463602
C	37.10679142591408	-24.61002026582199	5.55885987573550
N	37.05367669565258	-23.66092363472913	3.59478371721554
C	36.04833622844405	-24.57560610435052	3.68221287367382
N	36.05708856745137	-25.16329327914888	4.85778647491581
C	30.60450543602747	-24.47835238550181	2.25740397480451
C	35.50109171889675	-25.11924062907430	10.87739610242820
C	39.13606726602421	-30.08337590111940	5.80014385248792
C	33.78465427457001	-28.26350904390979	0.18095486382168
N	33.16821980961501	-25.50791599995405	4.80410104246635
N	34.56963587088176	-25.69409160608184	7.28402070995155
N	34.84997912334983	-27.51923711307181	3.70705408639103
C	32.91150109028470	-26.52268638646686	2.59192335896989
C	32.86656266219062	-24.02488081017175	6.73032714064543
C	36.25174787348328	-26.98052036748908	8.51774160430706
C	36.88491938522549	-28.81982074496100	4.09688884889393
C	30.64663773818568	-22.72948712718194	5.00450869685943
C	33.30285845148714	-23.05967782969817	9.64188800845175
C	38.64571858059525	-28.93199622380338	8.81082308802605
C	36.53464707989986	-29.70172913498795	1.15641312197358
C	32.54314816577591	-25.62544025579991	3.59118306370171
C	33.78285923227411	-24.61796094664649	7.59424121676150
C	36.72271041358781	-27.76478185402869	7.46826429216455
C	35.84449636555086	-28.36454409278164	3.29864545326898
C	31.49311539084297	-24.62660679923799	3.45692311118578
C	33.99763362659109	-24.20946215623954	8.97394959828604
C	37.86882384693222	-28.65933369435427	7.55654069040972
C	35.63505892724422	-28.77364529917334	1.91748346945414
C	31.51264864131384	-23.88944126243976	4.61077350754921
C	34.92128993257960	-25.07650592161859	9.49445154338763
C	38.07668157412498	-29.14203587441546	6.29189874187109
C	34.47709499677532	-28.17155017491869	1.50814652705921
C	32.56178653318391	-24.45858416154748	5.44366614637527
C	35.27589570913169	-25.99145917216910	8.42026105198133
C	37.04081375220571	-28.55623996451927	5.45298139181429
C	34.00953505700207	-27.37701033432329	2.63592235154559
N	36.23471025794871	-27.73449322747716	6.18855309621937

Fe	34.61522015535982	-26.71267831630310	5.53874858828987
C	33.53103028742868	-31.41031497560237	7.44273922630184
C	34.85349804620768	-31.64360085887941	8.15576368052805
C	32.20169768422032	-27.57593266229413	6.90921733562464
C	33.45383872781804	-27.92376709767013	6.15993517906309
C	33.72811832801155	-29.40452290110345	6.14371328476279
O	34.29735139253945	-30.02535629240042	5.27913545488133
O	33.26588907520438	-30.00027955374098	7.28622462057179
H	29.92927112540919	-22.47787162081875	4.21702184094710
H	31.23979854633835	-21.82764532251777	5.20766728028503
H	30.06978757243589	-22.94411965765671	5.91425578049886
H	31.18034220874182	-24.26820541895200	1.34571471588491
H	30.02635497592405	-25.39232959495359	2.06579972838535
H	29.88869063128546	-23.66062104045609	2.38654488295014
H	33.65088704410723	-27.27560017002043	-0.28032459637016
H	34.35238451353173	-28.87807985674468	-0.52470381675588
H	32.78573969474859	-28.71058663838867	0.27448385432529
H	36.21923949985747	-29.80121874753197	0.11295560603255
H	37.57454772470982	-29.34882990369917	1.15245097315794
H	36.53897431275255	-30.70873808467195	1.59473936216267
H	33.65496973284831	-22.91994397760028	10.66876903849847
H	32.21582047126623	-23.21151214600754	9.68687675448820
H	33.47180531998174	-22.11625000258974	9.10565007487195
H	36.59539201304631	-25.02671405836043	10.86248345424482
H	35.26821186666231	-26.06388180807630	11.38727914057058
H	39.47387441326858	-29.62373176014011	8.62763019722476
H	39.07429133181360	-28.01257233905839	9.23239648473490
H	38.01420013401620	-29.37706000232048	9.59154469793928
H	38.70220167811767	-31.01373334710120	5.41017906937649
H	39.72472620433428	-29.63835965917028	4.98683445367393
H	39.83432481224232	-30.35701621275492	6.59747621285013
H	35.11282557509239	-24.30789353399610	11.50107092048360
H	39.75001554896564	-22.96913452610908	4.36408443695558
H	38.66622659359780	-21.72002649655102	5.00183561524701
H	39.30194968088638	-22.97364568537692	6.07503888694607
H	34.86595806607357	-31.13339504333872	9.12242250432776
H	35.00584238515500	-32.71385293099333	8.32974666138311
H	35.68792621980622	-31.27109392078926	7.55844950133949
H	33.52346079385769	-31.88304744518215	6.45993889890845
H	32.69052965911344	-31.78533812056367	8.03022158871335
H	31.86033849130077	-26.56471445640489	6.70980177467347
H	31.38724926974182	-28.28363022957862	6.71605171503586
H	32.41755481864437	-27.65215582647762	7.98359329141628
H	37.25586916018504	-23.08042252798490	2.79364217227954
H	37.33010214350374	-24.92634269367842	6.56706761204675
H	35.34817433443497	-24.77802314651456	2.88507555171047
H	32.33015342363973	-26.50973815372691	1.67526052898944
H	36.73415358650349	-27.10466346635168	9.48222161779969
H	37.60308094072899	-29.49210737273250	3.63853463269284
H	32.30386403905692	-23.17932754161752	7.11306594875770

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B3LYP Scan/Melmid IPC Model/RKS/160 degrees Constrained Optimization

C	38.90578610320774	-22.73825251273004	5.04322487758987
C	37.74029855251068	-23.63519108051396	4.78131226077734
C	37.10754588794625	-24.57751763385093	5.55245004557463
N	37.04543242983880	-23.64769259014129	3.57948476580228
C	36.04991361474923	-24.57235959794431	3.67529991365865
N	36.06428725145151	-25.14869172669833	4.85629264215442
C	30.58438694819256	-24.53616700847307	2.28961545197427
C	35.53425743607740	-25.08920031926263	10.88186484550579
C	39.20642068072184	-30.01369375075703	5.79744176884727
C	33.78646603984966	-28.30535143959850	0.21485129986097
N	33.17678688690317	-25.52660233106434	4.82279291554442
N	34.59447193863219	-25.68632450318047	7.29457560761338
N	34.86935066945455	-27.52632473544804	3.72812957459333
C	32.90542212234939	-26.56610415690940	2.62459297705434
C	32.88831748264778	-24.02244933468626	6.73466133579791

C	36.28292434109279	-26.96157195273073	8.52865716959032
C	36.93953379459904	-28.77467209802828	4.10085106600248
C	30.65263179426790	-22.75022641186649	5.01201864262806
C	33.33460056509102	-23.03624532803818	9.63834277305460
C	38.69420671015527	-28.89181167420534	8.81571339280633
C	36.58174930676847	-29.67145007665977	1.16429482332863
C	32.53978377962638	-25.66128927041285	3.61782158520195
C	33.80856602485485	-24.60795697179561	7.59949730694115
C	36.75972577457723	-27.73914671821066	7.47669078690547
C	35.88074530030163	-28.34782872661641	3.31115291609494
C	31.48544673716154	-24.66746603527485	3.48185364695310
C	34.02706322685275	-24.19066135372978	8.97600774177886
C	37.91767319370081	-28.61919280517942	7.56125890089531
C	35.66765629993655	-28.76401139496961	1.93305038838916
C	31.51615815121959	-23.91438682012755	4.62527255871434
C	34.95101771253142	-25.05524174631577	9.50014971092901
C	38.13526187827790	-29.08856523053198	6.29367569535061
C	34.49083286508259	-28.19129814785752	1.53418660676856
C	32.57442874474673	-24.47066083923855	5.45495898463036
C	35.30360819286660	-25.97621991667680	8.43064847238653
C	37.09191384876251	-28.51283662326576	5.45736409603494
C	34.01641039282331	-27.40403953998790	2.66394242120173
N	36.27268479653792	-27.70790894918506	6.19715686591518
Fe	34.63786990411078	-26.71724455382262	5.55580163871516
C	33.33788949393620	-31.47909326221422	7.30324857187248
C	34.59202844208188	-31.75999601411857	8.11697361541287
C	32.23001216800021	-27.58143260367268	6.92462466593326
C	33.48608443186564	-27.93351712113414	6.18467991538742
C	33.75228532658179	-29.41693393150492	6.15786643229548
O	34.46544879547385	-30.01039760150121	5.38464363260792
O	33.09849907843446	-30.06278621656051	7.17480821364701
H	29.92555180741757	-22.51144714561719	4.22948755175661
H	31.24645201655645	-21.84442578789454	5.19462566089469
H	30.08702080956399	-22.95209281554508	5.93164488745824
H	31.14871410175508	-24.31953028748745	1.37218455461824
H	30.01864150546347	-25.45929875366651	2.10545428194887
H	29.85716738671122	-23.72920179595146	2.42281249891081
H	33.60163053440134	-27.32138028139021	-0.23670805717194
H	34.37271736739395	-28.88811367239981	-0.50261345302185
H	32.81029055821279	-28.79857202794138	0.31706570036954
H	36.25858853136022	-29.77990006557595	0.12411182525578
H	37.61279111754342	-29.29370925782864	1.14998741567420
H	36.61465044265498	-30.67749521911538	1.60361590003576
H	33.69012820778838	-22.88954712343841	10.66306207066486
H	32.24770937579336	-23.18764936789599	9.68795709343122
H	33.50188580969515	-22.09655081135693	9.09507968233258
H	36.62817998477000	-24.99273847528896	10.86390825685269
H	35.30615999885358	-26.03223178236395	11.39684184897939
H	39.52374393243404	-29.58178400780220	8.63212918160094
H	39.12107119520211	-27.97230534073827	9.23903235034476
H	38.06275914375989	-29.33896075746520	9.59521968140801
H	38.78246346330558	-30.94202449136848	5.39224143689801
H	39.79745687129169	-29.55320729496682	4.99441996578426
H	39.90107355083524	-30.29214416594932	6.59622070552621
H	35.14443344930425	-24.27635764860156	11.50258790070511
H	39.73265629220263	-22.91730993938033	4.34256588995266
H	38.63517682042584	-21.67591618753121	4.97178647824905
H	39.28570969886561	-22.91426632507953	6.05375251102248
H	34.53271310933302	-31.27890125315731	9.09690494907453
H	34.70973236455575	-32.83773544936891	8.26982707450461
H	35.47887771302813	-31.38846256015390	7.60078403569383
H	33.40898858293684	-31.91928083228461	6.30735465480663
H	32.44556799574923	-31.86117625331177	7.80287587674573
H	31.95525623904881	-26.53757746721672	6.81672402085575
H	31.38747525695258	-28.21195194562286	6.61559955819013
H	32.37835990239054	-27.79096788587935	7.99202070481406
H	37.24163563991949	-23.07230387061982	2.77316966858684
H	37.33384704512243	-24.88152240642381	6.56380079054245

H	35.35226553700692	-24.78946983095697	2.87977684225042
H	32.31570088753241	-26.56714541703689	1.71320723257516
H	36.76717232904844	-27.08309911187461	9.49253709122935
H	37.67120748698805	-29.42901395754298	3.63797005352679
H	32.32730780497319	-23.17355436521626	7.11243380540040

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B3LYP Scan/Melmid IPC Model/RKS/170 degrees Constrained Optimization

C	38.90244195320790	-22.69791513631599	4.99656353797189
C	37.73947674924519	-23.60354172588161	4.75424266480289
C	37.11396933329475	-24.53547757160887	5.54365443495616
N	37.04088690732751	-23.64047002303637	3.55513452970510
C	36.05086678399251	-24.56900670391343	3.67005723484131
N	36.07210685030056	-25.12471047432071	4.86068229581620
C	30.55996154883623	-24.61367354360670	2.33840365928064
C	35.58938232467509	-25.00998591832518	10.89087716688207
C	39.29246544771751	-29.92127013116406	5.82157395906438
C	33.77481758755478	-28.38688986058521	0.28707754023016
N	33.18701198782365	-25.5432449629332	4.85879054008317
N	34.62663783740795	-25.65891420133818	7.31857906684874
N	34.89452023158294	-27.53235504247810	3.77064997859870
C	32.90049606754280	-26.62049629822012	2.68046222121137
C	32.90639339306392	-24.01254440670840	6.75039453882114
C	36.33483259639208	-26.90478435386443	8.55352235430077
C	36.99835036128130	-28.72692203999328	4.13050563907339
C	30.64654538791729	-22.78139073890821	5.02918368276581
C	33.37229445796037	-22.98290400704629	9.63622414123397
C	38.77128212255165	-28.80160611523442	8.83866985991178
C	36.61458429934118	-29.67670078351055	1.21168097880361
C	32.53778588236801	-25.70312149581321	3.66317384840793
C	33.83763841589654	-24.58022573273360	7.61528025885911
C	36.81691487104378	-27.68046468221870	7.50261923906103
C	35.91844617052585	-28.33641162855456	3.34993100084142
C	31.47488195341072	-24.71934450147695	3.52267792903985
C	34.06417313126313	-24.14374185218511	8.98448786129150
C	37.98940377451776	-28.54121407845241	7.58501250945505
C	35.69369785183990	-28.77681082357529	1.98128179518399
C	31.51298345290769	-23.94688439509905	4.65304498501277
C	34.99556652927571	-24.99744280393224	9.51331101839646
C	38.21109187510675	-29.00844922999907	6.31783298057982
C	34.49829001936542	-28.23590146831419	1.59237412952145
C	32.58323734029444	-24.48244705420245	5.48062448240187
C	35.34568404997240	-25.92978710305876	8.45280918162542
C	37.15458826841449	-28.45362814552658	5.48404205042943
C	34.02437684357783	-27.44157887494266	2.71724876044254
N	36.32395639977342	-27.66136383468943	6.22564365602518
Fe	34.66812361340990	-26.70843418908562	5.59154531581159
C	33.11852187243161	-31.55823732308493	6.99834553226507
C	34.23747482940138	-31.97952938486283	7.93907755290944
C	32.28451553123330	-27.58749228621414	6.98594077417339
C	33.53129545827250	-27.93518433063579	6.22915389640658
C	33.77432716583310	-29.42154027755780	6.14507756172281
O	34.59907289291171	-29.98021882717347	5.46100592164952
O	32.94665371885149	-30.12650259054890	6.98031738417092
H	29.91558443980156	-22.55441933607776	4.24673132126169
H	31.23787854016155	-21.87147375487975	5.19869114263188
H	30.08506704165100	-22.97410836453807	5.95332076846311
H	31.11434022047122	-24.42454374029980	1.40901717679383
H	29.98646281831004	-25.53775457753436	2.18509746442710
H	29.83909910437702	-23.79908429359277	2.45919756842519
H	33.55563661370719	-27.41455221244216	-0.17410140299889
H	34.36404724817437	-28.96366486080743	-0.43279792993268
H	32.81421183540344	-28.90457664433848	0.41316232813398
H	36.27329347387614	-29.81373445347052	0.18069300518579
H	37.6355540358036	-29.27445445275433	1.16906241350768
H	36.68114993731178	-30.67264590798414	1.66975761394462
H	33.73681187916481	-22.81947281172284	10.65524165796087
H	32.28659568764773	-23.13830312898173	9.69827040743768

H	33.53029307056406	-22.05069371106841	9.07749201226080
H	36.68220188962515	-24.90368190594086	10.86360182534114
H	35.37381232278182	-25.94903664012278	11.41836348358878
H	39.60769490460818	-29.48339058192532	8.65572933281708
H	39.18901315531311	-27.87639305767265	9.25874254937299
H	38.14582943882596	-29.25298501922461	9.62058180460610
H	38.87881557735621	-30.85899904130681	5.42735880416807
H	39.87107147924691	-29.45908264229909	5.01054188276508
H	39.99661612479776	-30.18301598616769	6.61770590238173
H	35.19655690955321	-24.19364987710426	11.50508482532479
H	39.72822716783033	-22.88739722510468	4.29737096259289
H	38.62832619118335	-21.63794139846205	4.90615799255290
H	39.28538169053546	-22.85416516652970	6.00922352555458
H	34.05915170766773	-31.60225468712778	8.94955493783318
H	34.29688298270146	-33.07174947604536	7.98757464952889
H	35.19861619585573	-31.59964915672896	7.58928067273817
H	33.31207847855621	-31.90348486434295	5.98139667359026
H	32.15254593004877	-31.94257239695521	7.33126402671489
H	32.05702137586238	-26.52745345136254	6.96102263724359
H	31.42162460325673	-28.14992091557254	6.60887837173905
H	32.39629368408745	-27.89614196749241	8.03372180718452
H	37.23198264710419	-23.07854788465409	2.73815552447244
H	37.34539537149710	-24.82059857046120	6.55936296236633
H	35.35289884768274	-24.80445874347088	2.88002700327598
H	32.29916719394237	-26.64311830268807	1.77697340209798
H	36.82574304906310	-27.01433339818850	9.51545623344476
H	37.74034849647592	-29.36824975718049	3.66579827503579
H	32.34346611442155	-23.16164124208466	7.12070843327798

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B3LYP Scan/Melmid IPC Model/RKS/180 degrees Constrained Optimization

C	38.87503773576226	-22.63962709570332	4.94764311829325
C	37.72462686565237	-23.56627238799573	4.72581045080774
C	37.12162280552618	-24.49972201959789	5.53078886868632
N	37.01532768244748	-23.62677231139590	3.53402679266651
C	36.04144915767384	-24.56977662694793	3.66809503563037
N	36.08291619826176	-25.11274469995384	4.86401816834987
C	30.54300515357778	-24.70219842136606	2.39251857849330
C	35.65956853801499	-24.93555404474434	10.89917446120175
C	39.39529789218816	-29.82687985448189	5.84160110870734
C	33.78060561590646	-28.46429305440244	0.35573126846741
N	33.20612499669274	-25.56903672220410	4.89727620319348
N	34.66954315882129	-25.63955720063490	7.34480751608495
N	34.92433682601601	-27.55474790730176	3.81740218305657
C	32.90863658302891	-26.67940578276341	2.73682148973253
C	32.92788467120972	-24.01736810682402	6.77209147646162
C	36.40567942640424	-26.84734942819467	8.57655895602868
C	37.05353928131049	-28.70648843165003	4.16682067330445
C	30.63798562431247	-22.83287325810171	5.05730600206553
C	33.41014806936649	-22.94639203568719	9.64068271434544
C	38.88114823227981	-28.69055785824757	8.85311448171234
C	36.64810711516218	-29.70319747168162	1.26462938750561
C	32.54625202818146	-25.75240261865108	3.71064377564253
C	33.87288794639645	-24.56442625085248	7.63515983340234
C	36.89048062817835	-27.62335532139869	7.52736341601487
C	35.95536167099179	-28.34858713194780	3.39515875071115
C	31.47159278641953	-24.78201259629245	3.56823259771518
C	34.10723218645258	-24.10860732260912	8.99697343321735
C	38.08192177552605	-28.45798949361851	7.60503854323175
C	35.72187217929287	-28.80903456421649	2.03457296712740
C	31.51310437119663	-23.99395657198891	4.68781099861407
C	35.05175227463881	-24.94635610070945	9.52771237045779
C	38.29998828001916	-28.93241037954930	6.34040458875397
C	34.51489268918150	-28.28914277435091	1.65201118098648
C	32.59714743610725	-24.50698096773486	5.51149006213229
C	35.40184279772850	-25.88793653760992	8.47529077186360
C	37.22180888126420	-28.41032361401021	5.51345089138156
C	34.04200923122765	-27.48771834534995	2.77219344191131

N	36.38292039955017	-27.62706732203206	6.25642153489412
Fe	34.70690903540026	-26.70921182760691	5.63004669576246
C	32.88793495631586	-31.58350610113746	6.66491752475153
C	33.79049847775528	-32.14965667375558	7.75081293461498
C	32.34400689534049	-27.59113805619706	7.05104469278837
C	33.58031186498422	-27.94012796252066	6.27745118557949
C	33.78531587306652	-29.42838686672646	6.13178781058329
O	34.69526341341319	-29.98038851921245	5.55881862042720
O	32.79178528593177	-30.14754200083364	6.74565791918814
H	29.90064750960825	-22.62016969711856	4.27682060365098
H	31.22185353203454	-21.91603601149833	5.21472730480227
H	30.08327014745417	-23.02154679403519	5.98637437459119
H	31.08587856529842	-24.52556798507618	1.45396531115138
H	29.97361975553089	-25.63220634122261	2.26114550933027
H	29.81830647387617	-23.89014398446881	2.50731388529327
H	33.54438114773056	-27.50005621048502	-0.11392904732533
H	34.37020979310780	-29.04143734837947	-0.36354248382999
H	32.82802566201420	-28.99278902090261	0.49690289759731
H	36.29410719426537	-29.86216280616246	0.24108962988146
H	37.66048039649836	-29.28244678668909	1.20044469482895
H	36.74074181531900	-30.69062847223357	1.73631175670544
H	33.78153818721095	-22.76790628411400	10.65468030551535
H	32.32642775293310	-23.11070711826487	9.71341297326783
H	33.55526277041425	-22.01944062759524	9.06983352592090
H	36.74965868263386	-24.80682120168384	10.85984145353728
H	35.46911995597532	-25.87479080746260	11.43584319177103
H	39.72533759244428	-29.36255841810063	8.66970323425368
H	39.28971042266323	-27.75420289451120	9.25731363791520
H	38.27039886695068	-29.14105574567135	9.64706501664500
H	38.99735019756204	-30.77619964851396	5.45915205778893
H	39.95695700560065	-29.35980020819080	5.02142543411944
H	40.11195280463172	-30.06750405593055	6.63325285830884
H	35.25602197381659	-24.12283364539669	11.51116913877507
H	39.69616933181921	-22.82148424605115	4.24099385727145
H	38.58255567203707	-21.58508389505813	4.85143687920866
H	39.27159967904061	-22.78099498651413	5.95725477354577
H	33.44847722733473	-31.83882267094120	8.74159814466469
H	33.78285180505959	-33.24395788657536	7.71497994701842
H	34.81852100441139	-31.81080145664892	7.61291880055516
H	33.24978215994074	-31.85935043333514	5.67287188042340
H	31.85954708361366	-31.93045375502373	6.78210845764230
H	32.16068748472976	-26.52358454009219	7.09645013298850
H	31.46479044088563	-28.08922267918154	6.62569639199455
H	32.42576337976030	-27.97511664765774	8.07685775599698
H	37.18949372205680	-23.07022988114068	2.70960895869226
H	37.36734802817568	-24.76993369741954	6.54722209768552
H	35.33972661783640	-24.82431709702938	2.88736059632456
H	32.29831820101713	-26.72049928630801	1.84003298631357
H	36.90821896543839	-26.93963442932627	9.53426241230574
H	37.80215634352042	-29.33931556301366	3.70105539308246
H	32.35986663857103	-23.16744018718276	7.13685149324192

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B3LYP Scan/Melmid IPC Model/RKS/190 degrees Constrained Optimization

C	38.87238809219669	-22.62710120718282	4.85935565158040
C	37.71748547293742	-23.55646574185439	4.67602467452457
C	37.13793090825516	-24.48432854740284	5.50432461417556
N	36.97694619188267	-23.62780192844458	3.50405378268718
C	36.00883155070728	-24.57135990994078	3.67144263489941
N	36.08305526667773	-25.10464989901012	4.87022048898327
C	30.52294986073285	-24.79320709579535	2.45959992116841
C	35.73839096436346	-24.84282981243789	10.91175345511166
C	39.48137540319945	-29.75013351300648	5.87689683049882
C	33.77679873635985	-28.54966288439195	0.44200632451512
N	33.21727833295811	-25.59713215937179	4.95212672539162
N	34.71422841046755	-25.61140003376749	7.38074069688273
N	34.94811896136258	-27.58130132211638	3.87874803549633
C	32.91216426407678	-26.74023329552357	2.80852570069902

C	32.93977416317583	-24.02411660480158	6.80836619028834
C	36.48480466078850	-26.77338493957260	8.60602268395377
C	37.09696993609605	-28.69816127495266	4.21941344177181
C	30.61890707591045	-22.88971386771376	5.09977747158075
C	33.44188594514309	-22.90567282561622	9.65553807342899
C	38.98938056513204	-28.57541944543897	8.87698266613270
C	36.66380242836728	-29.75066715680836	1.33837446934190
C	32.54887944743816	-25.80428502059109	3.77375981296016
C	33.90433959443199	-24.54444312304575	7.66633585124367
C	36.96798493050050	-27.55566462183088	7.56102785859200
C	35.98205515709055	-28.37078873578145	3.45688380640278
C	31.46175619749554	-24.84843602644225	3.62876291769243
C	34.14851408761126	-24.06612382883973	9.01909918914742
C	38.17251925334807	-28.37157824443237	7.63539237415300
C	35.73730313426859	-28.85490967102815	2.10629140234805
C	31.50361059153147	-24.04592725525963	4.73817819405599
C	35.11278824746901	-24.88144573259592	9.54884841112766
C	38.38056920772164	-28.86244330014705	6.37569322980180
C	34.52175027291278	-28.35088225507069	1.72889529867934
C	32.60091414283459	-24.53528637147508	5.55843966317015
C	35.46442595652154	-25.83177007844876	8.50472174343901
C	37.28310383640257	-28.37008803249790	5.55571784252094
C	34.05339286501142	-27.53768843448352	2.84248487142354
N	36.44374834686362	-27.58557687255290	6.29751150291592
Fe	34.74494145177296	-26.70452312021404	5.68197745534661
C	32.72381666303954	-31.55494216625424	6.28488623117909
C	33.37466791277299	-32.26049728878898	7.46539631598209
C	32.39258759673126	-27.60368162976497	7.11366522892088
C	33.63322590702219	-27.94154868898426	6.34164741826558
C	33.80621993656822	-29.42515737972830	6.12898386779915
O	34.78536499075778	-29.98475471706870	5.69483691827025
O	32.67951923624632	-30.12686183875656	6.47384511137524
H	29.87558210615652	-22.69242583599827	4.32086839581182
H	31.19467097096615	-21.96569323954340	5.24439953303409
H	30.07068611451525	-23.07364063045567	6.03367353700486
H	31.05637609121822	-24.62206327502633	1.51460290664892
H	29.96265396309715	-25.73077712177301	2.34374676184717
H	29.79030321532826	-23.98770298876960	2.57022029506623
H	33.51681733449664	-27.59338501548647	-0.03121529915315
H	34.36989882563753	-29.11991661853260	-0.27995319252153
H	32.83621406438217	-29.09573549532946	0.59658578862864
H	36.30083599183856	-29.92578912363375	0.32057395708611
H	37.67162175058314	-29.32182388789141	1.25837549885706
H	36.77041759524970	-30.73125543827697	1.82130909899119
H	33.81959940079829	-22.71103276157464	10.66421929785121
H	32.36100291665495	-23.08290537581846	9.73927555479969
H	33.57038239875922	-21.98350598503866	9.07300163791271
H	36.82361938011410	-24.68206853841430	10.85687791137733
H	35.58320013950291	-25.78384405672119	11.45651993376626
H	39.83711721348664	-29.24316144997815	8.69435741770908
H	39.39438417346719	-27.62888359647186	9.26065208857674
H	38.39213840171090	-29.01801605290545	9.68550267647590
H	39.09061232495759	-30.70846342431852	5.50985166689915
H	40.03004259548466	-29.28672771467691	5.04581139352037
H	40.20815722558285	-29.97323514650643	6.66447797217456
H	35.31887031663211	-24.03846883476808	11.52400410823938
H	39.67404955011326	-22.81367990699419	4.13185910321252
H	38.57641879382672	-21.57351805666880	4.76335931845914
H	39.29673679152259	-22.76082925132181	5.85869695548051
H	32.85993563360775	-32.01464969175800	8.39804005832949
H	33.33024686748413	-33.34573116148351	7.32702327378217
H	34.42292431355051	-31.97153630309147	7.55643555242316
H	33.25688972448129	-31.77360779717079	5.35773143064066
H	31.67738985918400	-31.84642700451431	6.17649813338322
H	32.30552159750351	-26.54566245151424	7.33429686996457
H	31.50890377041299	-27.91634300105051	6.54237164745633
H	32.34650068920902	-28.17146137391746	8.05120996725048
H	37.12849712917226	-23.07820698824102	2.67055243265441

H	37.41167057264617	-24.74603280330034	6.51581005630075
H	35.28756121547789	-24.83395959773936	2.91147774777693
H	32.29311941795531	-26.79929780511967	1.91872006410139
H	37.00055466063256	-26.84531131444475	9.55842132151888
H	37.84708718565085	-29.33019197475581	3.75491558647564
H	32.36413854679217	-23.17732010277050	7.16852819026073

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B3LYP Scan/Melmid IPC Model/RKS/200 degrees Constrained Optimization

C	38.88995575017977	-22.65263773576356	4.72923594927207
C	37.71182877062276	-23.56283588485073	4.61020028661176
C	37.18014223845019	-24.50265001121522	5.45715263272904
N	36.88876407750394	-23.59791793743369	3.49302450187773
C	35.92246399304266	-24.53330571835903	3.70788603696857
N	36.07460181277739	-25.09538027720706	4.88607654368138
C	30.49767786699067	-24.89631165059121	2.53638936715334
C	35.82908937437284	-24.72421998635346	10.91927590381182
C	39.54748819178081	-29.70083784428235	5.93814727893096
C	33.77966706515600	-28.63609433885394	0.53740778501045
N	33.22672085725646	-25.62725518550325	5.01396561014490
N	34.75194958482944	-25.58398009042312	7.42510304861696
N	34.97398979400445	-27.60881615288075	3.94916269618088
C	32.92004374273367	-26.80187821861998	2.88636797756625
C	32.94289920744819	-24.03557757938398	6.85278317229629
C	36.56143139361009	-26.69204602412719	8.64232513283708
C	37.13284693773046	-28.70510888205326	4.28978881690084
C	30.58652767242749	-22.96054673264735	5.15271410953110
C	33.47553046095532	-22.85264670772491	9.66812399195994
C	39.08492499523891	-28.46457098448494	8.91761980547369
C	36.67899090961705	-29.81086431163483	1.42998352084718
C	32.55121183638719	-25.85962157916927	3.84391457613866
C	33.92863479123510	-24.52523455117352	7.70439684236047
C	37.03923576156308	-27.48877966193549	7.60628234873001
C	36.00812071121122	-28.39937171392682	3.53167528392713
C	31.44758637344399	-24.92324643973750	3.69772877868545
C	34.18849927604079	-24.01547653061025	9.04311096775411
C	38.25135533381511	-28.29304844881389	7.68220230700132
C	35.75399301862296	-28.90804181523897	2.19150784002890
C	31.48576155994808	-24.10758163134007	4.79791910597350
C	35.17678011519654	-24.80272774209192	9.57062932279425
C	38.44670532552218	-28.80980919862532	6.43105403992452
C	34.53308725688486	-28.41546748357134	1.81587176980943
C	32.59793349148536	-24.56922940704018	5.61392895127078
C	35.52519333964599	-25.76819913887251	8.53914154526843
C	37.33484405510533	-28.34353106853530	5.61496432616973
C	34.06953727920913	-27.58725117911017	2.92027477661277
N	36.49953040481751	-27.54838792488314	6.35011757183658
Fe	34.78143559573192	-26.70057218390912	5.74165952378563
C	32.63034688692398	-31.47308050484818	5.86577942153599
C	32.96517767666005	-32.33045122121079	7.07682596082393
C	32.44217964818649	-27.62865176173659	7.18303864990301
C	33.68695275784243	-27.94794787837531	6.40903283603816
C	33.83522480463291	-29.42115553200966	6.12710063026699
O	34.85205904919226	-30.00549479893235	5.83777869443685
O	32.62856913270836	-30.06840607282314	6.19132607156890
H	29.83554665496482	-22.78235702602804	4.37650865320095
H	31.14994567428971	-22.02691293544159	5.28358448937343
H	30.04688470518899	-23.14176913168305	6.09210994481363
H	31.02050706337407	-24.73413328772101	1.58393896231239
H	29.94653227049387	-25.84147066600260	2.43997071784197
H	29.75739690710093	-24.09703631001624	2.64127526399373
H	33.52088647638437	-27.68790423151706	0.04749006928666
H	34.36627888906607	-29.22240738935931	-0.17693703476053
H	32.83769985918161	-29.17508124795047	0.70752814878391
H	36.30660971796379	-30.00675595551214	0.41938093396691
H	37.68264520274598	-29.37621896428097	1.33149213830315
H	36.79828234635478	-30.78187080598087	1.92905145148974
H	33.86539905080404	-22.63430320336696	10.66729121224359

H	32.39839814369608	-23.04208877183573	9.77112690050382
H	33.58352675405754	-21.94002509697688	9.06665789440450
H	36.90850822734485	-24.53706243990130	10.83891509200723
H	35.70922133896239	-25.65909180543061	11.48312511846445
H	39.93539896919012	-29.12967108535841	8.73831185310228
H	39.48713549575209	-27.50730731413975	9.27691184103305
H	38.50080776471640	-28.89495851687589	9.74211041751449
H	39.15834357560045	-30.66805554199868	5.59345718409642
H	40.08558121251212	-29.25047916358187	5.09306104684900
H	40.28312687630201	-29.90517073881799	6.72263115428942
H	35.40162792641729	-23.92007251080091	11.52625627397287
H	39.63664195107658	-22.83698379507435	3.94481718199404
H	38.60365120565079	-21.59363034942750	4.67200152353646
H	39.38062874433112	-22.81036175411717	5.69415481054534
H	32.27829907036787	-32.12374772416501	7.90191506367436
H	32.88176629141070	-33.39201026236367	6.82199413700497
H	33.98551581921561	-32.14012796988984	7.41365328988158
H	33.33980940551763	-31.64684859836710	5.05482541080705
H	31.61812197378846	-31.67050582350682	5.50792591877841
H	32.40857224339761	-26.59853388270524	7.52246518836050
H	31.57245779206656	-27.80938882693220	6.53766488821445
H	32.31434957512921	-28.29847854578645	8.04200069606116
H	36.98842984296649	-23.03153113594741	2.66296266459189
H	37.52263847587631	-24.79247154937502	6.43959904862055
H	35.14557595179021	-24.77033477091633	2.99596076294830
H	32.29365099397388	-26.88010217370323	2.00320724979174
H	37.09195011406351	-26.73848472544778	9.58816475075073
H	37.88116522894619	-29.34324326338939	3.83078062733973
H	32.35781103708454	-23.19309907839250	7.20792444896385

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B3LYP Scan/Melmid IPC Model/RKS/210 degrees Constrained Optimization

C	38.86557367466647	-22.64053340878854	4.67369217734083
C	37.69253071440072	-23.56038253962426	4.58174793144724
C	37.18359194649680	-24.49910099777098	5.44382932656428
N	36.84870892022975	-23.60739091873537	3.48069675411588
C	35.89326916302293	-24.54821798953012	3.71871585972448
N	36.07149717967021	-25.10258004463731	4.89701834146721
C	30.47581266273366	-24.97472633329545	2.59982288099282
C	35.91761897775242	-24.62262698973288	10.91137152238368
C	39.58333197512366	-29.68940766088278	5.98400882174855
C	33.76897208420654	-28.70765237894101	0.61175651103818
N	33.23285407523415	-25.65304332480323	5.06158934460227
N	34.78280370644300	-25.56571999481498	7.45682102761103
N	34.98393486364178	-27.64257047328442	4.00482069408298
C	32.92110588344056	-26.85075689097274	2.94680597793350
C	32.94673066407210	-24.04793983905802	6.88820743094005
C	36.62780319530561	-26.62787800385492	8.66151612486201
C	37.14239752568973	-28.73822757144396	4.34795107014599
C	30.56142482712248	-23.01764888990160	5.19985203297100
C	33.51171111382663	-22.80934136028003	9.67311242555619
C	39.16442352428585	-28.37957295494279	8.93787574412095
C	36.66903870232534	-29.88105039562909	1.50417598076916
C	32.55098802265913	-25.90315361052550	3.89877804652394
C	33.95044418821249	-24.51287118322015	7.73239992313876
C	37.09501531602188	-27.44282696694603	7.63518305292640
C	36.01322062799618	-28.44180062871812	3.59213454808469
C	31.43521440036949	-24.98108596423194	3.75371317088806
C	34.22791534579492	-23.97484277242716	9.05671515933146
C	38.31073512461496	-28.24153054847826	7.71196986332071
C	35.74978045701793	-28.96783410870924	2.26046520019247
C	31.47144442014788	-24.15690952261324	4.84761162986613
C	35.23776973272133	-24.73766763552988	9.57897223413681
C	38.48743745435837	-28.78947340067874	6.47161277449051
C	34.52851264731690	-28.47541309827107	1.88463947464900
C	32.59570025363994	-24.59846192764651	5.65833110380502
C	35.57911293758326	-25.71813572888710	8.55897509923601
C	37.36214892203648	-28.34488949064857	5.66133934063502

C	34.07286818466059	-27.63265543936006	2.98095535222288
N	36.53709491269557	-27.53249368315506	6.38873738808306
Fe	34.80657312454562	-26.70304281644399	5.78628695436079
C	32.60193528516947	-31.36701221557981	5.53377243520872
C	32.66881980923883	-32.32523595949502	6.71255015023582
C	32.48543231144339	-27.64864706965582	7.25667154913795
C	33.72413638560173	-27.95317061671343	6.46724805694290
C	33.85273437764019	-29.41740043388917	6.14181009274601
O	34.87540589299103	-30.04145512975771	5.99379033713306
O	32.62150582835037	-29.99079060566518	5.96563774920442
H	29.80163026084829	-22.85571156102952	4.42865912899246
H	31.11469506595675	-22.07614728952284	5.31709419037367
H	30.03220141015006	-23.19636249349325	6.14562041825558
H	30.98909003225722	-24.81595127513870	1.64162922919445
H	29.93378079475196	-25.92637395306627	2.51658678993193
H	29.72818454078167	-24.18214580113746	2.70343294348454
H	33.51721415875011	-27.76414397289468	0.10926186265347
H	34.34812196657391	-29.30913689501778	-0.09601577874974
H	32.82264624452674	-29.23549660695165	0.79210312073692
H	36.28835969793315	-30.09133782273488	0.49956884824747
H	37.67144912852218	-29.44711837422049	1.39096789499587
H	36.79376254991743	-30.84490996394645	2.01556966803978
H	33.91413335997437	-22.57044450565162	10.66256890950557
H	32.43833338412016	-23.00825785071800	9.79545040603732
H	33.60098613241482	-21.90571187820341	9.05519717433279
H	36.99029647872634	-24.41147395845692	10.80405406204471
H	35.83252640599027	-25.55084503297205	11.49219828188485
H	40.01393965312802	-29.04661863451080	8.76149072900251
H	39.56939689771515	-27.41247043310775	9.26651696192550
H	38.59505306863762	-28.79082402481195	9.78214390571777
H	39.19083801660798	-30.66204967016215	5.65915347760097
H	40.11445847873068	-29.25357233586964	5.12689977532116
H	40.32567962213630	-29.88100432253926	6.76540819548435
H	35.48457799796401	-23.81912997836293	11.51524543195074
H	39.59878551604074	-22.82334508146269	3.87631044815371
H	38.56995056403883	-21.58410418109082	4.61632292603685
H	39.37551941880073	-22.78935941124138	5.62997361769457
H	31.86530952002686	-32.12174023608780	7.42543767329965
H	32.56378063101576	-33.35839980784444	6.36561304166947
H	33.62642566485962	-32.23430649806924	7.22810981699810
H	33.43297249390382	-31.53315015144356	4.84599207022725
H	31.66002648670732	-31.46791074875853	4.99138128090489
H	32.46213764983142	-26.62975125188505	7.63039966997478
H	31.61622191152023	-27.80031345843912	6.60380328086182
H	32.35217697564790	-28.34522216201674	8.09427401658669
H	36.92886310189791	-23.04521142603395	2.64569158740498
H	37.54633253293117	-24.78134948370483	6.42114394465229
H	35.10479075645257	-24.79427650069039	3.02285725206406
H	32.28872243275972	-26.94125585092822	2.06909756204171
H	37.17442781156623	-26.64998348694996	9.59905072117146
H	37.88473925873542	-29.38765410571203	3.89512281407122
H	32.35519756862948	-23.20859409794971	7.24018768230287

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B3LYP Scan/Melmid IPC Model/RKS/220 degrees Constrained Optimization

C	38.88320055853804	-22.68440003095786	4.60236780013392
C	37.69423506166049	-23.58623230456603	4.54306317578360
C	37.19161765436162	-24.51217858748199	5.42235775030247
N	36.82584045082807	-23.62841987444403	3.46112531171767
C	35.86307465011321	-24.55434124547965	3.72593675181654
N	36.05974656861544	-25.10373821051863	4.90372340513720
C	30.45286085467255	-25.01009105239755	2.64746357886606
C	35.96695613498633	-24.54516355358114	10.90901566411011
C	39.56910157153450	-29.71247460661930	6.03346003399941
C	33.73324343650035	-28.76152252800700	0.67803833256946
N	33.22651979379802	-25.65723202219853	5.09924720240560
N	34.79671385828995	-25.53814082278196	7.48033117515713
N	34.97575518011121	-27.65859060572992	4.04893372129790

C	32.90777033739218	-26.87322603988028	2.99528389992921
C	32.94162120124587	-24.04185477008079	6.91673272929789
C	36.66169756561238	-26.57508133152963	8.67672490414095
C	37.12827765600605	-28.76416511541909	4.39654569867407
C	30.54010349651004	-23.03691776141559	5.23478855515813
C	33.52702958107180	-22.76953641361639	9.68238588465686
C	39.18588738698308	-28.34370330815556	8.96526891630751
C	36.62955942190639	-29.94477353652771	1.57000562725015
C	32.53992004873864	-25.91909223854218	3.94178677389499
C	33.95762769923210	-24.49046737948045	7.75496578859830
C	37.11897434327380	-27.40618381298220	7.65899101095715
C	35.99735220942364	-28.47073903654127	3.64153860628940
C	31.41816569201567	-25.00410585213493	3.79649294435756
C	34.24617705923139	-23.93544011891685	9.07014082045044
C	38.32740023764699	-28.21543348468064	7.74169306844175
C	35.72147696593294	-29.01467717543967	2.31953749205710
C	31.45452650791889	-24.17355766073629	4.88551942433266
C	35.27024434004971	-24.68236549704880	9.58745815913842
C	38.48901194931635	-28.78839374050736	6.51082815388389
C	34.50149324530859	-28.51792201487888	1.94371581970816
C	32.58581185102969	-24.60341526531414	5.69300103271653
C	35.60759569344922	-25.67135692324893	8.57407983780276
C	37.36290313925335	-28.34595506655631	5.70011862587069
C	34.05807162040542	-27.65711299919296	3.03054239760185
N	36.55240321384840	-27.51112067720209	6.41772878072806
Fe	34.81599425823028	-26.68866430679252	5.82031259210413
C	32.71518321833989	-31.27395221138350	5.27528074761290
C	32.56801853365815	-32.29861730199996	6.38847360798511
C	32.50768962857141	-27.66249338337645	7.31095347763205
C	33.74912137508637	-27.94168840826197	6.51735987607718
C	33.89252785014273	-29.39883673263065	6.18013916287364
O	34.91030022334434	-30.04762407776104	6.18891798905784
O	32.69284549774061	-29.92288777929177	5.78400388361838
H	29.77570199702787	-22.88409478606077	4.46626974843778
H	31.08901850442242	-22.09177525216121	5.34298675567879
H	30.01644590483319	-23.21190225506258	6.18434235845886
H	30.96078772075517	-24.85844761653879	1.68528850854244
H	29.91261014923919	-25.96365628386822	2.57526008179315
H	29.70394165321205	-24.21832074065167	2.74801639018018
H	33.49394308855550	-27.82341064637941	0.15953587551544
H	34.30018957065074	-29.38440813527480	-0.02101238258280
H	32.77951670469747	-29.27105090713741	0.87136532028140
H	36.23866460862715	-30.16942140106883	0.57244380588707
H	37.63295050468720	-29.51778304540428	1.44046751161682
H	36.75483849551460	-30.90097072125204	2.09548816965371
H	33.93561984874993	-22.51962829231145	10.66658526025691
H	32.45600495907364	-22.97447163845940	9.81487699744885
H	33.60540711792635	-21.87053607712063	9.05625640212038
H	37.03440562625309	-24.31739648643324	10.78470093816671
H	35.90546044236604	-25.46967813721489	11.49865040431618
H	40.03261256719902	-29.01502793131053	8.79189457236514
H	39.59499743577093	-27.37470810032887	9.28290190262085
H	38.61865215756156	-28.74524049427718	9.81567390795025
H	39.16063153362862	-30.68576800048735	5.73096836118063
H	40.09997076669830	-29.30118903207114	5.16416878017125
H	40.31431886173525	-29.89899335843581	6.81336366383705
H	35.52928152855744	-23.74382722492462	11.51241540869624
H	39.59777257629485	-22.88795279746131	3.79318446590937
H	38.60359689474527	-21.62399473889354	4.53906729028077
H	39.40904596952787	-22.83152103433919	5.55026164032737
H	31.65628242903077	-32.12054068666325	6.96502953768575
H	32.51248167038730	-33.30721806167043	5.96581629146821
H	33.42374218206992	-32.26008283406998	7.06465640441169
H	33.64345307764646	-31.42477625878146	4.72198720033574
H	31.87347150406795	-31.31525890845378	4.58149853827245
H	32.46405021313958	-26.64416513043218	7.68565650191659
H	31.64217393146834	-27.83344193379786	6.65810390954888
H	32.39260969510946	-28.36191278249275	8.14988863169256

H	36.89580254371280	-23.07330425422663	2.62053021030104
H	37.57174529145647	-24.79400142770003	6.39306056718158
H	35.05674844588459	-24.79449955315613	3.04879213246189
H	32.27014402570204	-26.97217467986891	2.12227035752494
H	37.21666468678769	-26.58389351393938	9.60959278422495
H	37.86120457107480	-29.42945682068594	3.95145475427271
H	32.34620670722408	-23.20454724584157	7.26712354708736

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B3LYP Scan/Melmid IPC Model/RKS/230 degrees Constrained Optimization

C	38.88945810210774	-22.71060365508596	4.56775818446136
C	37.69344582158598	-23.60383844828509	4.52196952340985
C	37.19052017501377	-24.52082386457044	5.41033749529466
N	36.81740889034310	-23.64656753484998	3.44623898672037
C	35.85014047294852	-24.56419942486938	3.72304429700303
N	36.05119951607460	-25.10778319522166	4.90287773000821
C	30.43957339447865	-25.00486826410399	2.66989329131571
C	35.99860151359929	-24.50415284351480	10.90184802176815
C	39.52977703965963	-29.75832076173990	6.06164931645872
C	33.69539444751398	-28.77931850895229	0.70846985366782
N	33.21757082899828	-25.65114119900956	5.11717009285316
N	34.80140348468647	-25.52015047347294	7.48909274320223
N	34.95608670921826	-27.66774726883147	4.06973748942994
C	32.89153261088985	-26.87162264907347	3.01684940796700
C	32.93944139205063	-24.03084076287806	6.93152436248998
C	36.67569970217008	-26.54945798134368	8.6780006369260
C	37.09641671194532	-28.79578424758158	4.42227182867275
C	30.53252812086904	-23.02945798387715	5.25521012719999
C	33.54287229970684	-22.74260861858590	9.68620437340575
C	39.18152374928381	-28.34273183616769	8.97537509806312
C	36.57907498798615	-29.99053613950732	1.60364810074517
C	32.52837809841650	-25.91414125215738	3.96153462329144
C	33.96220159143960	-24.47326647430111	7.76482320480523
C	37.12191654579929	-27.39352602806217	7.66595185017303
C	35.96768722227267	-28.49513179919791	3.66636137607209
C	31.40705879082472	-24.99824976938131	3.81706016967978
C	34.26022289441213	-23.90994006245103	9.07452850885442
C	38.32022634170367	-28.21720000675594	7.75353463924124
C	35.68275641807637	-29.04561803518698	2.34910809245235
C	31.44550503245646	-24.16707993630729	4.90534573432499
C	35.29087410848956	-24.65087581306494	9.58715894539110
C	38.46720736982297	-28.80995848440755	6.53038281994278
C	34.46811279395224	-28.53632740766088	1.97164785293645
C	32.57875132487101	-24.59637642992045	5.71076767919038
C	35.62166868913078	-25.64541117080566	8.57673501372321
C	37.34341700297071	-28.36256506160431	5.71901595360386
C	34.03631187735281	-27.66359372394728	3.05328624145444
N	36.54878084523833	-27.50606322431942	6.42848736719298
Fe	34.81274493544321	-26.67822399146450	5.83384502584790
C	32.84539100545518	-31.22086417570765	5.12818030067957
C	32.58366290064892	-32.26732864844604	6.19957568231480
C	32.52983708906694	-27.67239092534967	7.37038763782578
C	33.75632511778516	-27.92925180832558	6.54813503706263
C	33.91568561442830	-29.38434922078424	6.21817699563602
O	34.91083273620984	-30.05078148604942	6.36743175657083
O	32.77339986768227	-29.87820634694691	5.65797798162427
H	29.76481012937835	-22.87896028320625	4.48954468705494
H	31.08184258532510	-22.08393973289976	5.35818467636105
H	30.01298153898180	-23.20157684724668	6.20753217310716
H	30.94569672481249	-24.85427426515933	1.70659261336610
H	29.89880284419952	-25.95827784549422	2.59959281227085
H	29.69119621972992	-24.21266561422571	2.77113691237668
H	33.46894365907996	-27.84213057323342	0.18254840081172
H	34.25294218082391	-29.41567775953179	0.01403149590444
H	32.73460137391023	-29.27349276123402	0.90649166484746
H	36.18178245612607	-30.21994761277929	0.60970132557473
H	37.58572591026754	-29.57383641828737	1.46610637047851
H	36.69850110387954	-30.94365895808289	2.13612607833124

H	33.95917485140785	-22.48580152769000	10.66539554193522
H	32.47363073915752	-22.94991072891002	9.82908923793313
H	33.61313434444833	-21.84700943789848	9.05427404748580
H	37.06462740410862	-24.27577254538347	10.76704621520680
H	35.94347596305040	-25.42483278158447	11.49812990750650
H	40.02362229860194	-29.02031386842377	8.80387905700411
H	39.59735270566251	-27.37428584675094	9.28575276156597
H	38.61426045746995	-28.73566514425346	9.82981215015410
H	39.10439394627732	-30.73088758726277	5.78075729373653
H	40.05955213601663	-29.37129914954403	5.18066083106971
H	40.27849207774663	-29.94144231173243	6.83900811293236
H	35.56485907050670	-23.69948631421097	11.50367376538316
H	39.59734708513265	-22.92505663948529	3.75553715439702
H	38.61753416653863	-21.64854052826337	4.49919197965520
H	39.42009104680568	-22.85555160659326	5.51331810809930
H	31.61543684064626	-32.10181016903215	6.67978052314869
H	32.57665421421616	-33.26738894999951	5.75365488405368
H	33.36374025382704	-32.23931826742299	6.96170164916657
H	33.82586521075861	-31.36303582019027	4.67093826212811
H	32.08052627087515	-31.24372846945519	4.35007779635511
H	32.42109617619431	-26.63244500804420	7.66330390633071
H	31.65017681525566	-27.97634382813576	6.78929174553414
H	32.52339347694701	-28.29882830600308	8.27426756180792
H	36.88543015404324	-23.09702819799091	2.60184990998864
H	37.57521306131469	-24.79956204511751	6.38007185050671
H	35.03770624428414	-24.80295892138711	3.05278175117700
H	32.25171733851720	-26.97018199298711	2.14536204372293
H	37.23653310068752	-26.55254350296793	9.60741262772050
H	37.81870987082286	-29.47644766584888	3.98302493440482
H	32.34461675208379	-23.19314331492138	7.28201800168347

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B3LYP Scan/Melmid IPC Model/RKS/240 degrees Constrained Optimization

C	38.88062319551920	-22.70591856256910	4.55100695930344
C	37.68845903197321	-23.60455841768023	4.51078182924843
C	37.18994055453739	-24.51882786371780	5.40439801862031
N	36.811151436419609	-23.65605525106841	3.43621111556536
C	35.84774780501615	-24.57555422593006	3.71870985850799
N	36.05196455741282	-25.11230572181675	4.90121455337905
C	30.42749192911404	-25.01468465397131	2.69512005574181
C	36.04599484280342	-24.46579323005716	10.88640321683813
C	39.50697059706552	-29.80052629974794	6.08091858080189
C	33.68211168912539	-28.78182765506845	0.72182122256728
N	33.21814812202052	-25.65039428364364	5.13079598907972
N	34.81487972179594	-25.51023519658674	7.49400375682604
N	34.95159399105190	-27.67420245673462	4.08119445580336
C	32.89077154037951	-26.86770630838167	3.02881445455157
C	32.93919050168897	-24.03391645710924	6.94840786835952
C	36.70395479574479	-26.52635982774967	8.67143689644961
C	37.07569357007378	-28.83099826981255	4.44207671020504
C	30.51490129555882	-23.04840895897473	5.28774212778331
C	33.56300289330152	-22.72910059581631	9.69070728720915
C	39.19908494584142	-28.33274649185380	8.97299644302678
C	36.54704258910333	-30.02897438465740	1.62670558428415
C	32.52691976155524	-25.91378469959820	3.97648681448192
C	33.97247089542263	-24.46709955677826	7.77360617494312
C	37.13755181188717	-27.38443865745891	7.66577574899866
C	35.95213791952803	-28.51813025393719	3.68307738679750
C	31.39922911398611	-25.00453350716155	3.83863655392163
C	34.28125721688063	-23.89487963581207	9.07708646677045
C	38.32877218518225	-28.21797440822248	7.75648034488034
C	35.66180598182999	-29.07009810174775	2.36769784635168
C	31.43519744925107	-24.17758691210978	4.93000768357129
C	35.32297377501014	-24.62574197090258	9.58156872757800
C	38.45874421736136	-28.83297584312553	6.54255845569686
C	34.45510816058000	-28.54509845516223	1.98614087561533
C	32.57481572330749	-24.60151809199253	5.72967103320818
C	35.64764645239670	-25.62468436199350	8.57334400591010

C	37.33375653382697	-28.38556895763863	5.73274435342929
C	34.03245167937428	-27.66416600153137	3.06463323112615
N	36.55381628829115	-27.50917650541567	6.43437397098320
Fe	34.81941347701425	-26.67313524859553	5.84082547355224
C	32.95624660574941	-31.19023436202467	5.03415982564205
C	32.46262741360353	-32.20698543563139	6.05050601632400
C	32.55417010640706	-27.68181622713432	7.40840219533578
C	33.76766267672754	-27.92329837158561	6.56345043712803
C	33.93429847363853	-29.37812837937017	6.24564195217422
O	34.88215571743841	-30.06636970778698	6.53714253355627
O	32.86329541069635	-29.83989548531869	5.54280054580354
H	29.74078145958516	-22.90350719625996	4.52746624701963
H	31.05670117749034	-22.09829221616081	5.38840778123003
H	30.00339486632155	-23.22642519134030	6.24331025235273
H	30.92871715055626	-24.85680661721418	1.73041194368475
H	29.89407187205313	-25.97212640915539	2.62359035910329
H	29.67330288134148	-24.22875427871544	2.80193260267241
H	33.46759059989255	-27.84321310098816	0.19347619060333
H	34.23380315808744	-29.42595370636649	0.02988018224272
H	32.71512929639587	-29.26434648115351	0.91851819652874
H	36.14795300311070	-30.25718120883388	0.63320638672602
H	37.55891455145211	-29.62528674513076	1.48865123592239
H	36.65448283349596	-30.98178398302115	2.16241316922533
H	33.98788075941179	-22.46502495129009	10.66427636323439
H	32.49667154813410	-22.94253653502619	9.84581432576423
H	33.62083880587868	-21.83607799300684	9.05391680629126
H	37.10789470458806	-24.22756339726808	10.73674794548360
H	36.00785791567178	-25.38389668598215	11.48795924897218
H	40.03274267000300	-29.01460882322941	8.80241082608173
H	39.62011253635306	-27.36218507428715	9.26936656045556
H	38.63741757612612	-28.71469401113333	9.83606229412482
H	39.06892251579151	-30.77339685531861	5.82123771854348
H	40.03274267000300	-29.43484889691366	5.18849494887816
H	40.26084596558916	-29.97782872280057	6.85463346356857
H	35.61207165306568	-23.66241498518344	11.48982630437562
H	39.58842288790393	-22.92080498613838	3.73883896731236
H	38.60378712554674	-21.64541153302268	4.47800694082192
H	39.41303460361593	-22.84417029218252	5.49655361489497
H	31.44183011052042	-31.97833736532215	6.36822071220181
H	32.46611083228440	-33.20996574633349	5.61109420986103
H	33.10964321590895	-32.21835820266639	6.92939732316123
H	33.99130422106769	-31.38709763217688	4.75128484123132
H	32.33402555693348	-31.18402406051927	4.13785287015619
H	32.42201672978905	-26.63922818695632	7.68221980334751
H	31.66833999091162	-28.02527159120654	6.85853515802076
H	32.59440080362814	-28.28752308549658	8.32576140041343
H	36.87643052293429	-23.11040905214070	2.58907704712551
H	37.57647675163275	-24.79101855935667	6.37521515374664
H	35.03513388712985	-24.82013998052647	3.05082835861614
H	32.24979418881817	-26.96483730086381	2.15800348032606
H	37.27358093800089	-26.52075768948249	9.59548325044253
H	37.78757009829987	-29.52592997211173	4.00815272119973
H	32.34130973647142	-23.19988253973409	7.30244085610394

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B3LYP Scan/Melmid IPC Model/RKS/250 degrees Constrained Optimization

C	38.87617321596122	-22.68622694430341	4.55836209668796
C	37.68803021832798	-23.58976795900356	4.51016461944471
C	37.18912621216128	-24.50798007573681	5.39943974646345
N	36.81569402607909	-23.64158598601651	3.43186917178356
C	35.85382311202186	-24.56496245818720	3.70810796771548
N	36.05507988641489	-25.10390538066264	4.89018071985145
C	30.42996951269150	-24.96956156544832	2.69194997571863
C	36.05890685556452	-24.48386474328979	10.88081297808491
C	39.47046754233835	-29.84558807601744	6.06367628294610
C	33.64659244750847	-28.76407832523151	0.71297918510248
N	33.21840591902289	-25.63017017388598	5.12385886408063
N	34.82261817531383	-25.50307564044455	7.48270009663319

N	34.94160853260703	-27.65879544396477	4.06321600318010
C	32.8860193779000	-26.83353961717811	3.01504194757401
C	32.94120502305395	-24.02774398002042	6.95407867204163
C	36.71636707897845	-26.52519888492678	8.64832540293966
C	37.04310916825886	-28.85560999796380	4.42958804727149
C	30.51751871916489	-23.02664386569036	5.30263548490569
C	33.56413006792381	-22.74868186783780	9.70876330055071
C	39.19689741375110	-28.35141582630191	8.94556914658984
C	36.48985624941429	-30.05749123294832	1.62051302380407
C	32.52702128968426	-25.88267951659720	3.96740523437709
C	33.97691617365561	-24.46605087999313	7.77377366835229
C	37.14093699162297	-27.38669293409689	7.64180012427774
C	35.92441839340050	-28.52551004219741	3.66990380670767
C	31.40104670020462	-24.97005607366826	3.83602294527374
C	34.28693572280219	-23.90429541246204	9.08152154888091
C	38.32287530107983	-28.23326091213231	7.73212347712181
C	35.62242300777033	-29.07986366675984	2.35805926243643
C	31.43727565390047	-24.15290311994574	4.93456496047616
C	35.33389308271661	-24.63439144267412	9.57600211896755
C	38.43818031233177	-28.85991172954804	6.52278320973064
C	34.42551134883111	-28.53444874360518	1.97498441575656
C	32.57650834573909	-24.58488657895092	5.73073795748088
C	35.65938933833663	-25.62353508279747	8.55847493004829
C	37.31511788566709	-28.40346029200769	5.71535741258431
C	34.02001617916364	-27.64080558168155	3.04967018811724
N	36.55039006091938	-27.51113331412801	6.41373234077027
Fe	34.82099269756092	-26.65890388740474	5.82377040679928
C	33.17475649569037	-31.26487631483360	5.10417091688917
C	32.40306343141800	-32.16658822896871	6.05391714914228
C	32.54655997690059	-27.67971560305260	7.37679936193361
C	33.77636935148588	-27.91152457189823	6.55309379401897
C	33.99085428015832	-29.37352729285088	6.31677914176579
O	34.87705278293132	-30.03487058770381	6.80194333152998
O	33.04417474500248	-29.87470194469879	5.48128146102568
H	29.74209829819251	-22.87593462410670	4.54483753097535
H	31.05933005847514	-22.07725950317825	5.40993808440860
H	30.00768049634812	-23.21237542601786	6.25763073954950
H	30.93176344764808	-24.80259241000697	1.72906184097630
H	29.89673362702772	-25.92638242227002	2.61101751898032
H	29.67553996870397	-24.18481963961259	2.80561578249048
H	33.45150391283492	-27.82512661217304	0.17763955751927
H	34.18400039060263	-29.42483111238372	0.02550591723546
H	32.66977322123020	-29.22429274757113	0.91417475312016
H	36.08358091886491	-30.28611525549114	0.63001200595878
H	37.50737180180094	-29.67052302474504	1.47591610903701
H	36.58476729646483	-31.00844538356919	2.16187325019124
H	33.98741928087357	-22.49500720117186	10.68578538164047
H	32.49852847045037	-22.96807388260020	9.86056772590676
H	33.61894355301906	-21.84761911820128	9.08310433765170
H	37.11857512052333	-24.23551426678283	10.73160245539471
H	36.02934526852174	-25.40934497328835	11.47138212865197
H	40.03183644245446	-29.03745201673103	8.77263632699853
H	39.62360047031264	-27.38275193619601	9.23985111078773
H	38.63613134225638	-28.73034113177789	9.81055738616604
H	39.01837551340218	-30.81585898986401	5.81838271769084
H	39.99392698632266	-29.49677802334310	5.16319794846095
H	40.22795769436031	-30.02391770104984	6.83358908602921
H	35.62011024628153	-23.69114740848390	11.49472222686736
H	39.58836803317234	-22.89514473267970	3.74849689674275
H	38.59491141391559	-21.62670883364849	4.48785262679337
H	39.40511688064983	-22.82530768423373	5.50573739356750
H	31.35314376953122	-31.86753203826097	6.11037033257697
H	32.44319449010416	-33.20429894557046	5.70686108653294
H	32.83163100047719	-32.12785734826754	7.05755157656600
H	34.23368096103263	-31.52491292940310	5.08613175413449
H	32.77504337387901	-31.31125732779902	4.09005485143028
H	32.38847721153221	-26.63517717366694	7.62914987210387
H	31.67560897998672	-28.04901093324398	6.81822421359784

H	32.58612647639423	-28.26948731451782	8.30422826971283
H	36.88184974119920	-23.09323743439968	2.58658946484652
H	37.57262001015442	-24.78094975574660	6.37121664968318
H	35.04427825764264	-24.81016532071882	3.03676055584097
H	32.24376729875284	-26.92410613936533	2.14444062946829
H	37.28977097094543	-26.52265327681315	9.57003568507874
H	37.74133191080379	-29.56584436710261	3.99811466135833
H	32.34272407453062	-23.19769792722856	7.31633935944226

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B3LYP Scan/Melmid IPC Model/RKS/260 degrees Constrained Optimization

C	38.86366853700310	-22.67551559325264	4.58266058137332
C	37.68404571302358	-23.58956148213279	4.52329798731165
C	37.18028875400815	-24.50698531873147	5.41069663957868
N	36.82639745484888	-23.65337968318715	3.43393580348927
C	35.86758563914974	-24.58215879487861	3.70242641253289
N	36.05701837197758	-25.11357997195883	4.88992093126457
C	30.43676691108246	-24.93160476745431	2.68367706220530
C	36.07487961074384	-24.48382323617206	10.87007109364517
C	39.43996881041998	-29.88041894537082	6.05968015827057
C	33.62329882462488	-28.75172627107017	0.70603346971214
N	33.21527590042613	-25.61942413224456	5.11930947298288
N	34.82006218550887	-25.50459474399837	7.47900516073818
N	34.92536150211391	-27.65778524246716	4.05717980348527
C	32.87967093314186	-26.81283537447057	3.00580372966793
C	32.94432474206315	-24.02108779029657	6.95428927554800
C	36.71443972779591	-26.53260992792777	8.63930091848009
C	37.00857966718561	-28.88539244226845	4.43070446218966
C	30.52773953249796	-23.00224118470995	5.30442193807825
C	33.57837325024690	-22.74503864232372	9.70788666098335
C	39.19095108686589	-28.36441816696141	8.93229679209677
C	36.44901745993058	-30.07847405200740	1.62038379962513
C	32.52531147240778	-25.86246274089025	3.96025140019967
C	33.97930749479777	-24.46451413853608	7.77234462666659
C	37.12965764383845	-27.40171360521401	7.63551535547763
C	35.89646677641559	-28.53922891793447	3.66815760065292
C	31.40493199055382	-24.94260647460334	3.83006903309747
C	34.29559078658566	-23.90303355325397	9.07866144112369
C	38.30829896316194	-28.25288664103160	7.72449226439603
C	35.59091338034062	-29.09107918477272	2.35592428280728
C	31.44282747407293	-24.13104339588195	4.93251735278372
C	35.34276538921892	-24.63538262722629	9.56933498056967
C	38.41310811770786	-28.88913708359694	6.51908600172134
C	34.40242983037290	-28.53044253784624	1.96930179336802
C	32.57816085093535	-24.57273125163156	5.72910712273041
C	35.66074384637708	-25.62692419030481	8.55166646607701
C	37.28804001597072	-28.43210473951894	5.71486106685849
C	34.00601424941804	-27.63052883244724	3.04235129336356
N	36.53151369370728	-27.53136432542986	6.41149738884170
Fe	34.80993793374463	-26.66050133165285	5.81819506965839
C	33.30625533775710	-31.29083848298828	5.11614757692360
C	32.44086448103013	-32.15404834124445	6.01962719365510
C	32.53415874690118	-27.66667338992082	7.38327555647424
C	33.75819367981025	-27.90622329123045	6.55302127760059
C	33.97868253509547	-29.37397532622497	6.36957145013581
O	34.76861305046641	-30.03180143624763	7.00466906280522
O	33.15343125771954	-29.88511490299322	5.42448381361363
H	29.75292187381742	-22.84578977009251	4.54720311243974
H	31.07325060983270	-22.05538062474485	5.41517349503705
H	30.01714718706575	-23.18943958550227	6.25872393163582
H	30.94187128617400	-24.76230906654838	1.72293573540338
H	29.89903466645066	-25.88538272265017	2.59654646656897
H	29.68589014860349	-24.143768856345034	2.79936493761322
H	33.44313515495478	-27.81152909848106	0.16759717907529
H	34.15253702491957	-29.42209017958615	0.02153997882551
H	32.63948122010133	-29.19700437933761	0.90654908674295
H	36.03963656471198	-30.30656232664292	0.63104951795248
H	37.46960247540841	-29.70048935435264	1.47319629520696

H	36.53688299552723	-31.02863054765411	2.16426802163466
H	33.99954973081206	-22.49831196471721	10.68759584228698
H	32.51073454427275	-22.95773238447850	9.85451438625358
H	33.64183483742335	-21.84163131893236	9.08633931017529
H	37.12978488445611	-24.21868805719365	10.71529580414320
H	36.06302827673350	-25.41378893468501	11.45394096881236
H	40.02268069640679	-29.05413082886432	8.75851018035490
H	39.62262720300591	-27.39469216959223	9.21562186410113
H	38.63567193325350	-28.73489074485503	9.80439300148363
H	38.98449424920775	-30.85138347772648	5.82332697373404
H	39.95854984774900	-29.53859571961054	5.15372709118373
H	40.20192724446566	-30.05558312048046	6.82587139629844
H	35.62912431457063	-23.70192693222160	11.49280498853786
H	39.58811865893852	-22.88170724499073	3.78303218642708
H	38.57397009158466	-21.61886851022928	4.50350638665691
H	39.38151644602534	-22.80538014407290	5.53743548865464
H	31.39338179340014	-31.84545299575256	5.96822396800721
H	32.50205089621730	-33.20289653520209	5.71157264628773
H	32.77577699405263	-32.08420837243077	7.05615189334785
H	34.36022091933053	-31.55606242998339	5.20718263872511
H	33.00521356422313	-31.37111020840236	4.07088535802986
H	32.36959553809309	-26.61862475240204	7.61622745757056
H	31.65880302448427	-28.05237951313097	6.84153941982277
H	32.59097043168564	-28.23898742814673	8.32026186232577
H	36.89914075145941	-23.10834053289569	2.58705842486583
H	37.55255449523697	-24.77138054972073	6.38918426433550
H	35.06856869758091	-24.83611925474863	3.02180739040604
H	32.2385958686789	-26.89647772389215	2.13363146403285
H	37.29226804788933	-26.52891616051135	9.55824223379324
H	37.69892848511547	-29.60367562699321	3.99976297267361
H	32.34980957982308	-23.18899973058622	7.31835545367530

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B3LYP Scan/Melmid IPC Model/RKS/270 degrees Constrained Optimization

C	38.87748432166212	-22.69594304318739	4.58419262095625
C	37.68762891655054	-23.59643516597342	4.52259666310531
C	37.17680729323388	-24.51401299233431	5.40575213385280
N	36.82639175280957	-23.64452136315646	3.43526079389355
C	35.85883952733578	-24.56508354813583	3.70061155088337
N	36.04610551564405	-25.10588824212229	4.88416405171125
C	30.42594759376477	-24.88449937658372	2.67417185769647
C	36.06444626581304	-24.49525462515547	10.86292761009463
C	39.37730697241259	-29.92747266782285	6.05401467450073
C	33.58162406291206	-28.72969922621173	0.69391376318032
N	33.19857308058793	-25.59826829223789	5.10927133684345
N	34.80517700066522	-25.49824640979529	7.46815418044856
N	34.90198339728401	-27.63546823085807	4.03759658162899
C	32.85731498655389	-26.78187289738984	2.99158453409676
C	32.93798536054188	-24.00234063815343	6.94776051317877
C	36.69001587171650	-26.54442014305292	8.62826826129004
C	36.96871750873736	-28.88984066061812	4.41444174811020
C	30.52864074535642	-22.96305537034324	5.30063420601835
C	33.58010614670395	-22.73695171140350	9.70386737868720
C	39.13739829894895	-28.41358037365740	8.92859259145808
C	36.40092607060637	-30.07415016611245	1.60371572423566
C	32.50776840648390	-25.83275169313461	3.94918933976701
C	33.97073778027622	-24.45395561410036	7.76423988688816
C	37.09776018682249	-27.41679048795440	7.62440202661443
C	35.86385789335529	-28.52626625596904	3.64917890773559
C	31.39314673979690	-24.90545367654702	3.82120640908478
C	34.29053851476680	-23.89761689136154	9.07176513137473
C	38.26342076391024	-28.28496262772448	7.71630024940450
C	35.55228998184329	-29.07763501431463	2.33800246619300
C	31.43593453961670	-24.09725845696180	4.92591465477124
C	35.33282435867797	-24.63795989633447	9.56090673132987
C	38.36423230414077	-28.92055665465774	6.51000345015249
C	34.36746393341382	-28.50895967870719	1.95294056079039
C	32.56810653545078	-24.54872425457296	5.72149930397204

C	35.64449892085413	-25.62912833496776	8.54099431899242
C	37.24989401524684	-28.44508669391329	5.70171016677396
C	33.98024223345540	-27.60410043790042	3.02543294857598
N	36.50273683758251	-27.53577229606876	6.39743717192895
Fe	34.78932486511333	-26.64861494449442	5.80324097485062
C	33.56356899505993	-31.34727226936615	5.19661614508939
C	32.60241322653281	-32.17952202654863	6.02976788906383
C	32.51956198010691	-27.65778877346035	7.37533075701195
C	33.74418597372618	-27.89558192563909	6.54552117273643
C	34.01206980112170	-29.36310828019105	6.43878404934371
O	34.70251539874695	-29.97463507839916	7.22095543839501
O	33.35332931299980	-29.92995586709946	5.40355357448256
H	29.75573941592912	-22.79855870557990	4.54318053592674
H	31.08093597404564	-22.02054228408233	5.41482372318019
H	30.01578742934245	-23.14946286537602	6.25387217670456
H	30.93270785466937	-24.71425950331945	1.71447114015429
H	29.88289691690980	-25.83488529633885	2.58288007958991
H	29.67933904741952	-24.09298060423903	2.79241025070648
H	33.40184220557936	-27.79002452081388	0.15445594289947
H	34.10502154094390	-29.40340331112318	0.00819930670874
H	32.59747647692872	-29.17130101396387	0.90093142352933
H	35.98715761391267	-30.30269894786370	0.61630823183865
H	37.42410191024328	-29.70477799817090	1.45261848333702
H	36.48284658323070	-31.02304857066919	2.15083119817943
H	34.00421444014743	-22.49362487807243	10.68316256174072
H	32.51169208154001	-22.94462315980076	9.85210884866407
H	33.64688148114541	-21.83300362622004	9.08345438627664
H	37.12276217719871	-24.24307140289212	10.71003760128300
H	36.04011601535942	-25.42498792878504	11.44679975979784
H	39.96169398210664	-29.11257103618650	8.75643644305989
H	39.57921638070124	-27.45070213047921	9.21947377261061
H	38.57189378212048	-28.78170141587626	9.79507251370750
H	38.90795425068566	-30.89118604622543	5.81473292005826
H	39.90534210794159	-29.59347186421821	5.15062252230034
H	40.13286434516185	-30.11527640251266	6.82350385799203
H	35.62706043152797	-23.70794416587987	11.48480289060075
H	39.59718010446502	-22.90509729212327	3.78105177791658
H	38.59940511140487	-21.63563571057175	4.51271884223168
H	39.39669934074515	-22.83778434849334	5.53653447969065
H	31.56546392101962	-31.90051241689731	5.82439452339789
H	32.72120288817381	-33.24240270160924	5.79554054655841
H	32.79675991920016	-32.04282253213223	7.09503685289875
H	34.60158102510774	-31.58443156321311	5.43382223836651
H	33.39953547594374	-31.48786498705690	4.12752697413447
H	32.33053583468943	-26.60632403337816	7.57177836888894
H	31.64693420078579	-28.08260065175860	6.85762535023020
H	32.60248478368573	-28.19553522612882	8.33008285474101
H	36.90257686997150	-23.09509570633869	2.59152787355962
H	37.54927773165112	-24.78824290705467	6.38145042818509
H	35.05539950052158	-24.80698610973886	3.02078005697780
H	32.21484481632060	-26.86098128893494	2.12000347871745
H	37.26569913765206	-26.54837092368473	9.54853763326861
H	37.65106060879432	-29.61556253035354	3.98310147305005
H	32.34878708113281	-23.16751421014859	7.31417287514591

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B3LYP Scan/Melmid IPC Model/RKS/280 degrees Constrained Optimization

C	38.88400538525025	-22.72120485521494	4.59310611672363
C	37.68696485139424	-23.61165767661634	4.52545920317289
C	37.17001986474030	-24.53275846538191	5.40134235943478
N	36.82395189093238	-23.64344297907591	3.43894321605444
C	35.84936340516820	-24.55836136638086	3.69769746005367
N	36.03390020760592	-25.11101468319866	4.87623337153298
C	30.41630487145027	-24.82559658365881	2.65847242387204
C	36.04239120648671	-24.53184299776995	10.85861476001764
C	39.31602568131628	-29.97082831375636	6.02964812208219
C	33.54184831325414	-28.68906568259880	0.66509513925767
N	33.18037347677971	-25.57603076515051	5.09231135470179

N	34.78657591597825	-25.49887149359064	7.45252667321053
N	34.86752950005452	-27.61996513511900	4.01501656331221
C	32.82809864930442	-26.74954538987257	2.97201378885950
C	32.93848293325675	-23.97956930139051	6.93322463248351
C	36.65418965361138	-26.57469010243350	8.61482339554922
C	36.92189823337332	-28.89681374415847	4.38740632083614
C	30.54305334773377	-22.90770855587555	5.28685216568619
C	33.58625571829798	-22.73498031324146	9.69734359256434
C	39.07902016142764	-28.47461206751918	8.91413570844520
C	36.35522616261332	-30.05076344307200	1.56623015025667
C	32.48691016609250	-25.80003218649504	3.93225832683885
C	33.96374216404342	-24.44643568079055	7.75068174334290
C	37.05477371389225	-27.44872531523397	7.60931865111517
C	35.82398215510734	-28.51416202137149	3.62189048454028
C	31.38310043351396	-24.85950183828695	3.80547618357139
C	34.28605230908641	-23.90017026409468	9.06167547156653
C	38.21100278137189	-28.32921251681240	7.69955936104191
C	35.51103837302117	-29.05482220238035	2.30648423676663
C	31.43625542859989	-24.05264827735061	4.91067280167308
C	35.31705708615267	-24.65594638551818	9.55120668119020
C	38.30952708641582	-28.95886215155890	6.48950476391029
C	34.32933533418206	-28.47847895281349	1.92465306648250
C	32.56305149208247	-24.51893736956495	5.70556850984644
C	35.62047030033655	-25.64608795534889	8.52779454268358
C	37.20261110379803	-28.46771247079928	5.68058504630914
C	33.94634546048649	-27.57820794093676	3.00274158996334
N	36.46161632719565	-27.55610777653353	6.38023417582215
Fe	34.75948415656613	-26.64414566785265	5.78464131032807
C	33.85778015336975	-31.39730606148010	5.35960254781142
C	32.80109321115695	-32.22231970130171	6.07621770947612
C	32.47630316747835	-27.63119024591384	7.35079581556119
C	33.71421804321289	-27.88141260234304	6.54459640906349
C	34.03538178946235	-29.34263779160579	6.55353270805330
O	34.59469664275471	-29.89193093340066	7.47574078648289
O	33.58192814392837	-29.97915033352461	5.45378542020118
H	29.77324506057965	-22.73178021376397	4.52886488665184
H	31.10713407492768	-21.97254514927246	5.40367892792034
H	30.02673752537920	-23.08962559276166	6.23908297340895
H	30.92434944333373	-24.65366865951267	1.69971913652720
H	29.86678919000519	-25.77172934746304	2.56205705845605
H	29.67502141322066	-24.02971922606027	2.78089961294393
H	33.35708423568155	-27.74448652451926	0.13610076694282
H	34.06654857588627	-29.35326102461915	-0.02885324786074
H	32.56002637893103	-29.13707286475701	0.86954677887053
H	35.93950068639142	-30.27275944213905	0.57816187603574
H	37.37967842049372	-29.68450635264574	1.41594565876935
H	36.43436338951727	-31.00295685250082	2.10812095604552
H	34.01994244314836	-22.49134521685452	10.67235904098918
H	32.51825409095311	-22.93774417062787	9.85542789469966
H	33.65145139404983	-21.83285931652688	9.07422328270088
H	37.11189305648547	-24.32778638159101	10.71309238159657
H	35.97226010188017	-25.45378906911546	11.45128709419461
H	39.90637365674225	-29.16838207477788	8.73560738457320
H	39.51618147249382	-27.51512387003951	9.22235249672504
H	38.50941201243837	-28.85771678463842	9.77140072499017
H	38.84129184394071	-30.93071060891339	5.78521095182045
H	39.84671152481539	-29.63615939430188	5.12809889659095
H	40.06974942208117	-30.16709905953786	6.79877327941767
H	35.63400838085951	-23.72002036786884	11.46861505807288
H	39.60182202996979	-22.93030549763121	3.78826313992798
H	38.61425576417950	-21.65826959070198	4.52925395476013
H	39.40235034615607	-22.87386436160858	5.54425480599550
H	31.80255671803859	-31.99298752097248	5.69456987668861
H	32.98692532252119	-33.29011697150123	5.92162525583889
H	32.81992016312189	-32.02678640286233	7.14973456851418
H	34.85231665724873	-31.58705938260447	5.76535680755567
H	33.86334169292736	-31.59500830050581	4.28697150566689
H	32.20937016319769	-26.58041588254848	7.41479919869864

H	31.63068913249304	-28.18936892216641	6.92231660197398
H	32.62190953947815	-28.02902480188748	8.36471638034066
H	36.90340370754603	-23.08728144184510	2.59992639935722
H	37.54155293862399	-24.81801750238802	6.37424917783304
H	35.04342485534259	-24.78849553240694	3.01673975377990
H	32.18537641087065	-26.82088525288188	2.09993432243457
H	37.22618244354810	-26.58936021045171	9.53723766519515
H	37.59922142838672	-29.62411438123093	3.95070961275995
H	32.35895342377533	-23.13865801360756	7.30111593984682

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B3LYP Scan/Melmid IPC Model/RKS/290 degrees Constrained Optimization

C	38.92448610986137	-22.80878466338109	4.59443765285993
C	37.70502060042021	-23.66795077081784	4.52333728275656
C	37.16742154647606	-24.58333401854578	5.39278346229464
N	36.83885382294507	-23.66902811384949	3.43883800010446
C	35.84228970341746	-24.56128680726457	3.69263415878540
N	36.01602841376958	-25.12862021145386	4.86575092160931
C	30.40379350187210	-24.70543802625240	2.63733537242935
C	35.99592035246901	-24.61651322068851	10.86270637383384
C	39.23341272937760	-30.00854421916844	5.95836408348771
C	33.44873110838755	-28.62720583233684	0.62680910525591
N	33.14946464364130	-25.53212408308575	5.06762337176325
N	34.75146616077671	-25.50757427303805	7.43269155848255
N	34.79699692680108	-27.59683395324693	3.97972392469288
C	32.76918682159081	-26.68928759788551	2.94456478975805
C	32.93920885440864	-23.94375568354914	6.91899318234722
C	36.58786405093744	-26.63784327963293	8.59504937094982
C	36.84142710950939	-28.89644008382454	4.33206359196201
C	30.58100825610372	-22.79710069816684	5.27056875914515
C	33.58703647494730	-22.75372279872969	9.70637790815248
C	38.99490713004680	-28.56651586640675	8.87078060199169
C	36.25294042538080	-30.01886905286523	1.50327529592949
C	32.45038781530970	-25.73464831871422	3.90758397383566
C	33.94650372007856	-24.44446979050637	7.73892008975164
C	36.97801599141278	-27.50819307142357	7.58183586730063
C	35.74519036041802	-28.49484519930131	3.57481837093935
C	31.37005371686801	-24.76646298863826	3.78351820423028
C	34.26959282594287	-23.92293760225432	9.05961249294658
C	38.12765713038786	-28.39757822367523	7.65866053663136
C	35.42348412511244	-29.01919309616127	2.25480225923377
C	31.44427636082478	-23.96371315527705	4.89051655123535
C	35.28091523870070	-24.70619996870698	9.54688157898507
C	38.22474186148736	-29.00694185458798	6.43701932258376
C	34.24506824006820	-28.43085250927306	1.88290276812241
C	32.55837889887341	-24.46158386400347	5.68413651571639
C	35.57324175153298	-25.68823388912720	8.51268629290129
C	37.12077985709547	-28.49755890275183	5.63551773107063
C	33.87403397861792	-27.53598584085792	2.96977401387808
N	36.38173310391008	-27.59647804837175	6.35228077260415
Fe	34.70147200601408	-26.63975902996319	5.75959870260099
C	34.39087949483430	-31.41673032046721	5.78256317994564
C	33.22933408452693	-32.31461992314544	6.17544603048234
C	32.31164546445653	-27.59759816146482	7.18743352984126
C	33.63358219429001	-27.85190629905595	6.52984557453296
C	34.04747358167477	-29.27256854298599	6.75913861763120
O	34.38515371134671	-29.68067198453204	7.84882058588918
C	33.96932306339328	-30.03796226200938	5.65400407499938
H	29.81558783414422	-22.59931558225085	4.51362801817967
H	31.16909004233429	-21.87716611630777	5.38975248718389
H	30.06076412421651	-22.96856504974395	6.22257721722398
H	30.91510910965232	-24.54219186235431	1.67882930893589
H	29.83199891854465	-25.63801707437663	2.53813325488883
H	29.68149946947290	-23.89285610276742	2.76341288378959
H	33.26678441054956	-27.67792555106789	0.10532314917228
H	33.96456399173125	-29.29032717458089	-0.07470091699109
H	32.46533596703514	-29.07037013672254	0.83446324810605
H	35.83858174638092	-30.21701352386744	0.50959660879368

H	37.28517183359067	-29.67046358379800	1.36450949723373
H	36.31014473015641	-30.98168264667018	2.02926151264122
H	34.01941357534416	-22.53023856539077	10.68677081394140
H	32.51473688436236	-22.93950241187709	9.85589521688138
H	33.67189456679432	-21.84491854041610	9.09538901963395
H	37.07194116953753	-24.43982783848238	10.72995020153775
H	35.89468755777957	-25.54311321602318	11.44334806463174
H	39.81555275615987	-29.26608114566459	8.68392311998092
H	39.44160141202553	-27.61507761447303	9.18997173712417
H	38.42146644601546	-28.95358250004573	9.72362609475148
H	38.76118831923218	-30.96156529631973	5.68401959506506
H	39.77084016716547	-29.65018017200847	5.07000640904097
H	39.98126867098782	-30.22543588463992	6.72760538686798
H	35.60357860673953	-23.80087471325456	11.47817056135713
H	39.63476922594123	-23.03047048995158	3.78626753552434
H	38.68177681313266	-21.73890469331709	4.53872812013740
H	39.44121283223974	-22.98125119274866	5.54309784755330
H	32.40041457366767	-32.20885950002024	5.47050043770139
H	33.54520362130453	-33.36288784366345	6.17530289926109
H	32.87055933953640	-32.06831318002377	7.17678180312737
H	35.19911348741171	-31.46935312056615	6.51273327672511
H	34.77995728645637	-31.67095815055830	4.79571314010299
H	32.00271062657190	-26.55756679094529	7.14800866708136
H	31.53409596390517	-28.21628815934671	6.71435210457432
H	32.36482450159655	-27.92427051157716	8.23426767898439
H	36.93012482129631	-23.10791898081129	2.60431370904434
H	37.53412131858694	-24.88539355656354	6.36251060224714
H	35.02978679934045	-24.76671265819999	3.01155692583909
H	32.12422105106671	-26.74517123566271	2.07298875078863
H	37.15504603348574	-26.67230577557654	9.51983475621690
H	37.51613257090899	-29.61753821679760	3.88103358596402
H	32.37756048827934	-23.09341363212069	7.29278296267394

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B3LYP Scan/Melmid IPC Model/RKS/300 degrees Constrained Optimization

C	38.92450216555459	-22.83440190249532	4.59948589547541
C	37.70354836167107	-23.69119437668232	4.52515061093885
C	37.16318536319183	-24.60806683194754	5.39143133753746
N	36.83768438377053	-23.68658209936791	3.44042797134317
C	35.83869589436806	-24.57701832967552	3.69117670114333
N	36.01045485529157	-25.14852621768206	4.86248578100078
C	30.38855748261360	-24.69893895150707	2.64082730238937
C	35.98141925921073	-24.65083176125040	10.86319706394001
C	39.23754193280273	-29.99136453944426	5.92330111635761
C	33.42889518829671	-28.61803741469527	0.61394608735522
N	33.14083684515182	-25.53222179960856	5.06078889403901
N	34.74109330048692	-25.52047870028149	7.42644657722760
N	34.77284578693205	-27.60490397459670	3.97399929217906
C	32.74511829043029	-26.69390969943329	2.94324440221300
C	32.94888035248461	-23.93586607096968	6.90752370950211
C	36.56119646203199	-26.67258262199113	8.59391494316684
C	36.82813091519202	-28.89210304335079	4.31190158328563
C	30.59403079856681	-22.77721680328179	5.26283618148526
C	33.60122115633576	-22.75590435285756	9.69905915904884
C	38.98202869160369	-28.58800204237679	8.85309732281215
C	36.24456248997435	-29.99523325755349	1.47615802094300
C	32.43492442303727	-25.73527959952629	3.90512463921214
C	33.94851620544658	-24.44767161964891	7.73028995319950
C	36.95085177696475	-27.53988890444798	7.57774756664885
C	35.72723940509614	-28.49271965719565	3.56074824792792
C	31.36080758009489	-24.76004150434877	3.78186321152839
C	34.27226859364603	-23.93215308808144	9.05318882116720
C	38.10926238287784	-28.41859593753050	7.64482264627213
C	35.40814939716271	-29.00826830251622	2.23669110258268
C	31.44702969832966	-23.95173510375187	4.88396454918008
C	35.27076401476990	-24.72944957908445	9.54429414328866
C	38.21283169911491	-29.01276130968559	6.41578853872829
C	34.22465289859776	-28.42643152599101	1.87111043075119

C	32.56100271688158	-24.45403035335951	5.67497268475784
C	35.55567781908749	-25.71337812958796	8.51001508799874
C	37.10216438109111	-28.50805191902198	5.62078474847878
C	33.84963740367794	-27.54124885624781	2.96470583504974
N	36.35242288500350	-27.62451303770450	6.34831506731394
Fe	34.67845708230935	-26.65402011968830	5.75499621072982
C	34.50476361762347	-31.39517487468662	5.88227095785723
C	33.32419842050686	-32.30966777145969	6.16359890274947
C	32.29793137618217	-27.55082356433143	7.22443483508975
C	33.59791530178028	-27.84491826298139	6.54030537994698
C	34.00107650973266	-29.26319995985097	6.81154072472180
O	34.19296134875653	-29.67859993723350	7.93456865110377
O	34.08157519753274	-30.02290082084968	5.70398710634925
H	29.82640655363610	-22.57751825110999	4.50868453280585
H	31.18917141429037	-21.86097645050107	5.37506023845266
H	30.07726153780902	-22.94096198573361	6.21807274162056
H	30.89550505592973	-24.54392277081863	1.67864580240852
H	29.81070915308519	-25.62860492976132	2.54989197163857
H	29.67192269219370	-23.88135547215027	2.76669956736251
H	33.24444245950538	-27.66637446516686	0.09768681443562
H	33.94667263645420	-29.27584131555047	-0.09111927317066
H	32.44674376054027	-29.06509925221444	0.81897603186246
H	35.83052879418221	-30.18897756919535	0.48148213086690
H	37.27371237295781	-29.63725569020882	1.33864588881010
H	36.31024545614357	-30.96161972851266	1.99449879175189
H	34.03038021753658	-22.54094095054068	10.68274594674545
H	32.52573661885446	-22.92837514429817	9.84138203241466
H	33.70158097442741	-21.84645030093915	9.09138524771941
H	37.05860543825046	-24.47724792323212	10.73530773182337
H	35.87469024891472	-25.58089871021249	11.43712495167234
H	39.80598599141830	-29.28201088701381	8.66014820834166
H	39.42461001642451	-27.63538690842267	9.17455037734579
H	38.41428072055665	-28.98166247706875	9.70669960399892
H	38.78185436279368	-30.94800331023800	5.63422269729438
H	39.76898761321697	-29.61040081452878	5.04075086690313
H	39.98888184623100	-30.20695194521542	6.68950626784629
H	35.59011697214073	-23.83778257575995	11.48271358010015
H	39.63402836296484	-23.05355198366143	3.78996113791167
H	38.68341505764709	-21.76389911451674	4.54859443219859
H	39.44149122007962	-23.01170051851016	5.54711386215375
H	32.56436003640852	-32.21415855693327	5.38340320063041
H	33.65478255138481	-33.35303367140133	6.19179031619458
H	32.86991804762996	-32.07070327792645	7.12696876649835
H	35.23882619556372	-31.43228749824727	6.68788949007674
H	34.99196064356226	-31.64667260705964	4.93940829225594
H	31.99822173744776	-26.51033452007740	7.15259708620660
H	31.49837950022708	-28.17924740269701	6.80348856069621
H	32.38266287252733	-27.83725266986164	8.28018373135744
H	36.93024924877582	-23.12242534030555	2.60808032084095
H	37.52871025294649	-24.91356194270386	6.36059892485576
H	35.02551854349847	-24.77767277635866	3.00948388790558
H	32.09773576825359	-26.74802374179618	2.07336558633956
H	37.12695442185020	-26.71197533560453	9.51936828404185
H	37.51095963223153	-29.59932988805421	3.85115330462314
H	32.39609787324120	-23.07897688903008	7.27952176814434

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B3LYP Scan/Melmid IPC Model/RKS/310 degrees Constrained Optimization

C	38.92988677728500	-22.86570067226496	4.57818522457326
C	37.70121177737082	-23.71221633409229	4.51441043489815
C	37.16080731144703	-24.62478295757202	5.38526014266980
N	36.82667819601625	-23.70118156461166	3.43669060704795
C	35.82311161565497	-24.58412001076167	3.69581306092596
N	36.00003637816845	-25.15668527362759	4.86570469879613
C	30.36072920830925	-24.71784349341039	2.66590793407360
C	35.98149909889917	-24.64732763033996	10.86533600583705
C	39.23899934015812	-29.97604226508892	5.91836351715003
C	33.39591067935283	-28.64451670982570	0.63907447308448

N 33.12820946954525	-25.53955323429952	5.07228651723382
N 34.73642107258760	-25.52155400794193	7.43138921349655
N 34.75648857640790	-27.60968846001965	3.98552173824707
C 32.71431650585761	-26.71773324849280	2.96784255833220
C 32.95956535499560	-23.92274015606268	6.90338571282649
C 36.54509798132284	-26.68498797427898	8.60540023640046
C 36.82951035611521	-28.87207764913139	4.30824880381411
C 30.60201716941883	-22.76494727320293	5.26184313770299
C 33.62749071960689	-22.72948896144138	9.68556960152994
C 38.96388802358764	-28.60534075756641	8.86198787751039
C 36.23693283282486	-29.98397903782848	1.47824520925991
C 32.41221663397182	-25.75124368780046	3.92441581558613
C 33.95622478824085	-24.43762689812614	7.72797711222511
C 36.93545290484823	-27.55060354809993	7.58778849450278
C 35.71973683694407	-28.48393460070967	3.56445844562991
C 31.34227568673353	-24.77158893594569	3.79933038265643
C 34.28488629404701	-23.91786094677058	9.04785069797093
C 38.09634218804151	-28.42642661963342	7.65127751822877
C 35.39586455905128	-29.00481676809754	2.24359154667060
C 31.44323276144443	-23.95043333981176	4.89067923291836
C 35.27225014676925	-24.72500249374529	9.54561615767257
C 38.20830930743065	-29.00637493445511	6.41596503674592
C 34.20075100158034	-28.44036143988751	1.88847701060073
C 32.56004718924546	-24.45082968698915	5.67882649486419
C 35.54746168488524	-25.71768128146748	8.51712980995145
C 37.09833700208186	-28.49913401947936	5.62150064882442
C 33.82449801161390	-27.55784641313706	2.98394221951195
N 36.34065368088842	-27.62854224626502	6.35575915430035
Fe 34.66357252087236	-26.66238015642498	5.76582383069525
C 34.59840226966898	-31.37257864070959	5.91326456219656
C 33.38802632354903	-32.28994894620295	5.97383030916106
C 32.31261325133559	-27.52134957825568	7.28573773046643
C 33.58531440990861	-27.84606923842815	6.56504389399402
C 33.97103123558522	-29.27240781713836	6.84050222270232
O 34.01858386117288	-29.73098061504066	7.96309343752656
O 34.20430303944956	-29.99407278946067	5.73000955190156
H 29.83065888285019	-22.56795826403171	4.51082702172142
H 31.20517393012123	-21.85223808661395	5.35897728656034
H 30.09084100471660	-22.91340057525983	6.22253963169737
H 30.86020798420579	-24.57529538169629	1.69791631271139
H 29.77790761225414	-25.64570221352855	2.58965828510734
H 29.64889337689314	-23.89569748481390	2.78924739052178
H 33.19706596642150	-27.69653998712881	0.12138061035963
H 33.91426553307341	-29.29938640599459	-0.06828519797175
H 32.42027394981346	-29.10095167437583	0.85424979036862
H 35.81738937581099	-30.18385284029853	0.48707881621732
H 37.26129665785749	-29.61584429081554	1.33239092038872
H 36.31608135497176	-30.94857498230315	1.99811172887090
H 34.05941836373006	-22.51252094239682	10.66759207477349
H 32.55016720112422	-22.88867132352455	9.82936809953456
H 33.73804846513478	-21.82558336894534	9.07142745383823
H 37.06132342474761	-24.49048184536667	10.73830636704975
H 35.85998043517952	-25.57146577016678	11.44588675539735
H 39.78771329517856	-29.29914831685794	8.66781649264827
H 39.40637053595873	-27.65558128056269	9.19194994749805
H 38.39209009210014	-29.00395464218587	9.71060698367909
H 38.78824091953499	-30.93181896887101	5.61879585519760
H 39.77211394708239	-29.58477289385855	5.04138165339269
H 39.98829067557531	-30.19568106030636	6.68541271588090
H 35.60102723584540	-23.82410420537826	11.47814505374126
H 39.63112448239089	-23.09202177969356	3.76341682908829
H 38.69767178098522	-21.79322833148534	4.52783439207402
H 39.45279643300599	-23.04638977438058	5.52192109142621
H 32.76068170175520	-32.16468998882505	5.08748938160983
H 33.70887118715363	-33.33567354875711	6.02060448470666
H 32.78714706040797	-32.07910680765243	6.86077555022818
H 35.20086354490513	-31.44962610594100	6.81888751535361
H 35.22286430719490	-31.58866499239035	5.04548950910378

H	32.02902288094931	-26.47696134220265	7.20995124470537
H	31.48750056703273	-28.13921175807975	6.89995660803870
H	32.42565460434976	-27.79886548532846	8.34060636921584
H	36.91707946789294	-23.13818898964683	2.60330797822776
H	37.53173567876473	-24.93290942976982	6.35157859768798
H	35.00342686228301	-24.77952599064774	3.02035972488959
H	32.05975254579352	-26.77944044650607	2.10386535312842
H	37.10836756978060	-26.72748497929375	9.53223213020302
H	37.51999926685259	-29.56728050094685	3.84057695039392
H	32.41622078902692	-23.05723572222793	7.26926991781964

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B3LYP Scan/Melmid IPC Model/RKS/320 degrees Constrained Optimization

C	38.92446291630103	-22.87584356467594	4.57949323848835
C	37.69587037882903	-23.72250904174161	4.51584530274326
C	37.15673184993726	-24.63685355573907	5.38567197256297
N	36.81977811028961	-23.70948438311684	3.43939425572551
C	35.81662820069322	-24.59301200724111	3.69845779144663
N	35.99526524728143	-25.16780146675655	4.86688440004256
C	30.34502667165278	-24.73241164313627	2.67872790836856
C	35.97575140344654	-24.65948768102799	10.86743654665923
C	39.24957872213629	-29.95734737731955	5.90416905087820
C	33.38422139064694	-28.65437009481760	0.64406138570903
N	33.12251709680972	-25.54857674053795	5.07509865795698
N	34.73330009415783	-25.52984242301897	7.43151281643030
N	34.74547465876041	-27.61786668424641	3.98969827238254
C	32.69569208866786	-26.73656216530546	2.97914924305972
C	32.97185624999958	-23.91719439052361	6.89501317677960
C	36.53113699045520	-26.70380946370212	8.61129711621308
C	36.83317220998393	-28.85909798241314	4.29977021950115
C	30.61385369543455	-22.75786139657814	5.25586175510415
C	33.64717600206896	-22.71931814039784	9.67389354524457
C	38.95650016511392	-28.61794634844225	8.86042684671954
C	36.24364353176225	-29.96476306814461	1.46737949880848
C	32.39919236027851	-25.76556289161013	3.93275352940777
C	33.96395715443055	-24.43660099660391	7.72232228555769
C	36.92396271939715	-27.56498194889758	7.59063962827269
C	35.71734094696106	-28.47911695145362	3.56133249253682
C	31.33331397164498	-24.78163418588933	3.80645800231464
C	34.29411468989068	-23.91622100764266	9.04150919020816
C	38.09007409491331	-28.43456196007003	7.64950805855511
C	35.39417571274050	-28.99838892398588	2.23969139760737
C	31.44574476920611	-23.95153959026294	4.88989667357027
C	35.27054996855659	-24.73293552619815	9.54530722531241
C	38.20961236100282	-29.00116650678387	6.40863311790623
C	34.19096146395341	-28.44677198315242	1.89167443280158
C	32.56407206228609	-24.45163905845629	5.67596920913174
C	35.53934438863143	-25.73077217915657	8.52022644470610
C	37.09761664181170	-28.49477749402309	5.61635660724996
C	33.80994293715514	-27.57146470325361	2.99135815525848
N	36.33190718906700	-27.63722096582746	6.35686553792454
Fe	34.65171372793969	-26.67560676165644	5.76978861630753
C	34.64578071315542	-31.36147331192418	5.93790531750428
C	33.42264546341369	-32.26489650159655	5.91458602048067
C	32.32510652571680	-27.48754797492336	7.33451755645047
C	33.56809529647906	-27.84884252634886	6.57909693486624
C	33.91499261321530	-29.29047352237531	6.84827343658788
O	33.80808270433978	-29.80069314638602	7.94544731902362
O	34.28813478846268	-29.97400340274944	5.75244524130446
H	29.84054898830208	-22.56140612134381	4.50675107400657
H	31.22339783256993	-21.84846914189681	5.34355986200107
H	30.10598446133546	-22.89598601700017	6.21983285423303
H	30.83902889319208	-24.59850104859024	1.70670195601890
H	29.75871600198748	-25.65883340250605	2.61276914484117
H	29.63671992319656	-23.90702665981983	2.80061838165433
H	33.17639390405107	-27.70668645635178	0.12938210059863
H	33.90597130784315	-29.30325545544567	-0.06629595888454
H	32.41290887893385	-29.11920570062194	0.86070677126227

H	35.82281778724627	-30.16566112545933	0.47697029073770
H	37.26312661375552	-29.58423697172597	1.31922597932691
H	36.33575324864972	-30.93024017426708	1.98344790206253
H	34.07938124854159	-22.50324606839925	10.65598081715096
H	32.56811966686904	-22.86763090475914	9.81624001011354
H	33.76761473209480	-21.81864399718258	9.05688409613892
H	37.05788765665338	-24.51649324137884	10.74386099899627
H	35.84063251950881	-25.58001331354397	11.45073874452664
H	39.78220754399395	-29.30878262804904	8.66369901180454
H	39.39634588786669	-27.66890477169944	9.19598551645017
H	38.38478636786822	-29.02217961653615	9.70646725709803
H	38.80772291165749	-30.91389924669399	5.59406664271403
H	39.78142819917112	-29.55284367995513	5.03244070519565
H	39.99888490765639	-30.17816458886764	6.67085947250314
H	35.60335289264470	-23.82948601999625	11.47604073784352
H	39.62472811053824	-23.10060026248559	3.76345253801263
H	38.69194817465810	-21.80333917688165	4.53127212379053
H	39.44865872123363	-23.05798361100686	5.52224357679993
H	32.85258843733462	-32.12179767249121	4.99272595239083
H	33.72941054797397	-33.31468515463723	5.96675028763501
H	32.77258249211435	-32.05653352667876	6.76577970853702
H	35.19417200260745	-31.46182241135874	6.87542790656550
H	35.31616147550191	-31.57487603417849	5.10453872928093
H	32.06686659308883	-26.43675134220985	7.26286190438118
H	31.47258385710883	-28.08393113095369	6.97567244751759
H	32.45701224624718	-27.76719299994771	8.38604374672566
H	36.90888912635597	-23.14473818976256	2.60704085485998
H	37.52907053034396	-24.94665987486584	6.35094398313765
H	34.99587923141559	-24.78721721482813	3.02391527444463
H	32.03708355128855	-26.80209422287752	2.11855701573266
H	37.09188778803676	-26.75001258611483	9.53947909541967
H	37.53089166547803	-29.54289348816391	3.82600115305336
H	32.43659711900650	-23.04455720135654	7.25581760165001

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B3LYP Scan/Melmid IPC Model/RKS/330 degrees Constrained Optimization

C	38.93215435042364	-22.90589114292196	4.55758518745488
C	37.69889013396224	-23.74632229925979	4.50142532805952
C	37.15881172077348	-24.65544312594648	5.37616835951496
N	36.81871324970174	-23.73265248248704	3.42829714954238
C	35.81259962056849	-24.61092510125443	3.69424736598371
N	35.99308258010384	-25.18285227930091	4.86367617190868
C	30.32945617105944	-24.74754677276778	2.69464394794145
C	35.96482975717289	-24.65754831882787	10.87430506055762
C	39.25547514125186	-29.93771423379041	5.90316920796933
C	33.36069973470747	-28.68037401715841	0.66677301364649
N	33.11681387867452	-25.55552534906921	5.08239921388727
N	34.73240412104888	-25.52917137935219	7.43502248937140
N	34.72709576013328	-27.63438890534997	4.00712151656295
C	32.67085335600606	-26.76254318411782	3.00185516129136
C	32.98767577440363	-23.90305508406369	6.88498835118284
C	36.51683449371036	-26.71315298606784	8.62427715444818
C	36.83192250672256	-28.84894787080527	4.30413006185581
C	30.63207408445043	-22.74256726937990	5.2445542225289
C	33.66668413716473	-22.69649174011744	9.65900901769817
C	38.94714585918422	-28.62439432036669	8.86900051474595
C	36.23901317641038	-29.95968670882920	1.47303569833322
C	32.38438996479733	-25.78089484601141	3.94746537747804
C	33.97380981144779	-24.42609905356482	7.71702272773394
C	36.91151695568257	-27.57236343728785	7.60215580155458
C	35.70725512363475	-28.48349311572351	3.57219771679101
C	31.32493280141034	-24.79068816220636	3.81627123750325
C	34.30445340301169	-23.90251461277004	9.03453828267051
C	38.08159260620485	-28.43733344791789	7.65802210560882
C	35.38271116808109	-29.00461642611883	2.25180898867775
C	31.45211507984931	-23.94717426595180	4.88768411079497
C	35.26885054347276	-24.72813286064097	9.54726471605840
C	38.20808203893042	-28.99227502139699	6.41257874174879

C	34.17093473959733	-28.46665479775700	1.91112845615749
C	32.57105902476115	-24.44679504943042	5.67309695231627
C	35.53225457348542	-25.73322453064371	8.52786840981735
C	37.09406046094465	-28.48723062609841	5.62201612150565
C	33.78695990201324	-27.59521093312062	3.01272954837465
N	36.32258744770707	-27.63974840028747	6.36704164433517
Fe	34.63869649516164	-26.68802325729733	5.78322146734033
C	34.70578802033180	-31.35054551279544	6.02698708742767
C	33.50199562022189	-32.23340503789908	5.73770680983800
C	32.31846649050541	-27.45028472087526	7.36569301544561
C	33.54896706998879	-27.84671928608411	6.60628391876330
C	33.84495879400927	-29.30368859983760	6.87689363364253
O	33.55721045364855	-29.85637193841755	7.92072513797356
O	34.39828687498901	-29.95269762309035	5.83831664137417
H	29.86260559874556	-22.54237122879062	4.49252414659659
H	31.25106634641732	-21.83925657820216	5.32809271896052
H	30.12072773991392	-22.86953498834600	6.20824545037206
H	30.81693251655157	-24.61737849846233	1.71876805303968
H	29.74375642280501	-25.67480221619526	2.63679086569583
H	29.62099037515798	-23.92244470549275	2.81755056776287
H	33.14617125556273	-27.73446250588316	0.15152220599802
H	33.88320156791145	-29.32763421231459	-0.04449926864677
H	32.39256645013315	-29.14980476030584	0.88748510815720
H	35.81855148538419	-30.15825941020077	0.48197196963765
H	37.25497705292608	-29.56963374918833	1.32573478974605
H	36.33975921592736	-30.92728537579810	1.98340717225345
H	34.11300842741741	-22.46675712177481	10.63165010250715
H	32.58975334434196	-22.84249957528944	9.81914934124087
H	33.77838949727285	-21.80499323130489	9.02744637240252
H	37.05326279861725	-24.56722389800231	10.75826852067663
H	35.78190031609013	-25.55727604190764	11.47707540040750
H	39.76916611955405	-29.31968234355005	8.67238337746259
H	39.39220852693215	-27.67748705565721	9.20385176452151
H	38.37409000006062	-29.02526877939120	9.71571745811990
H	38.82132674346892	-30.89584335276554	5.58701806693459
H	39.78494005614363	-29.52403592359995	5.03431240760761
H	40.00597352482782	-30.15743679392493	6.66900010836011
H	35.62582313737409	-23.79766977171952	11.46059809257361
H	39.62887481099913	-23.13799426017485	3.74056749684397
H	38.70526255986702	-21.83238130183873	4.50523080481727
H	39.45803154133370	-23.08663572646400	5.49967139761857
H	33.11353319936505	-32.04154054962129	4.73412260939170
H	33.78679697905311	-33.28883679006126	5.79850440157964
H	32.70649295519738	-32.05409277715924	6.46291379235709
H	35.06961506837212	-31.49905212076939	7.04461665384252
H	35.51743195681817	-31.53845937433363	5.32268432009934
H	32.07029854897822	-26.39963635164446	7.26802855339611
H	31.45555338006774	-28.04877636426362	7.03869185632283
H	32.45784005242538	-27.69982926751367	8.42374114943554
H	36.90729143605965	-23.17092296358602	2.59383518677231
H	37.53374651235484	-24.96426053398827	6.34080269270480
H	34.98816604039407	-24.80285710052456	3.02344365793342
H	32.00763005794905	-26.83360502668857	2.14526358916480
H	37.07470181211887	-26.76185873114651	9.55408418781650
H	37.53654703666731	-29.52268832245674	3.82606045195221
H	32.46068944591831	-23.02248627823894	7.23853326042267

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B3LYP Scan/Melmid IPC Model/RKS/340 degrees Constrained Optimization

C	38.92721791453156	-22.91608072763856	4.54248018374151
C	37.69496608741417	-23.75856151916138	4.49458160672432
C	37.15914932642893	-24.66425652719241	5.37552531373047
N	36.81083327163618	-23.75096776037675	3.42464686238951
C	35.80693121047563	-24.62947237472777	3.69849135957176
N	35.99232999909702	-25.19560172907303	4.86985191392294
C	30.30962383310497	-24.78994518099268	2.72712920071734
C	35.97992748263498	-24.63043691023936	10.87696134101705
C	39.27401661017928	-29.91454138551093	5.92081799784527

C	33.34508124054308	-28.72573379522477	0.70786388273391
N	33.11712555295794	-25.56890754692764	5.10038692074499
N	34.73843283652594	-25.52681185034004	7.44719356687680
N	34.72034564947715	-27.65510928189432	4.03650009716045
C	32.65355413144477	-26.80151617469424	3.03860252738493
C	33.00661477836721	-23.89233829992043	6.88182619535732
C	36.51589107269116	-26.71091531102666	8.64506878730696
C	36.84063038694903	-28.84387569674954	4.32452248814288
C	30.64178260122803	-22.74731676219480	5.24358408760880
C	33.70173811314860	-22.65933471207453	9.64065404961453
C	38.95336146629278	-28.61248849865531	8.88979471069995
C	36.24524518642475	-29.96699741763922	1.49806352787128
C	32.37438298773688	-25.80895891623476	3.97488806209734
C	33.99093813494838	-24.41297581353973	7.71737886173227
C	36.91103997139067	-27.57148291329857	7.62406873117093
C	35.70804841356446	-28.49344027782489	3.59756303222397
C	31.31584547996936	-24.81847496788474	3.83957901833071
C	34.32710540060275	-23.87844017410939	9.02909488629159
C	38.08639527530548	-28.42966209500718	7.67913021684957
C	35.38109856509639	-29.02219686173330	2.28090166675435
C	31.45543097562596	-23.95922914309805	4.89696890667184
C	35.28268546715618	-24.70861489158645	9.5509993871667
C	38.21811957200634	-28.97955286777941	6.43213458307572
C	34.16005903517693	-28.50030945371525	1.94709170190934
C	32.57954497437537	-24.45057301960643	5.68001808773264
C	35.53661372808437	-25.72649924140362	8.54190310273036
C	37.10070658832416	-28.48064292444570	5.64230085270519
C	33.77407008911424	-27.62861158718000	3.04787721066465
N	36.32351650859480	-27.63982871310074	6.38886304542366
Fe	34.63535923511414	-26.70010003969873	5.80716513325819
C	34.68852130371423	-31.35096565815169	6.01829613545386
C	33.52789255767286	-32.17283460771039	5.47907129953300
C	32.33207911638796	-27.41741222993164	7.42014670297920
C	33.53438684069620	-27.84741829444129	6.63340698069606
C	33.74639083312436	-29.33187875725004	6.84631528671705
O	33.27890004268327	-29.94217922385634	7.78898353664723
O	34.45131328317345	-29.93533143733182	5.87463529601334
H	29.86775898854440	-22.55449580189590	4.49432935753739
H	31.26433107151734	-21.84511076721911	5.31080360939530
H	30.13684701038359	-22.85993791142266	6.21240455233388
H	30.78757771345163	-24.67162965809432	1.74505008893989
H	29.72432009265049	-25.71832330446642	2.68664615925090
H	29.60160310939831	-23.96396599219068	2.84654837124999
H	33.12543801605561	-27.78423968933934	0.18666100250572
H	33.86661192511198	-29.37662291648238	-0.00079152163364
H	32.37942768968415	-29.19648485903243	0.93619002245378
H	35.81977708413481	-30.17502145253691	0.51108705066493
H	37.25386956091298	-29.56192528687902	1.34118648486611
H	36.36501604062568	-30.93115811078010	2.01067125297163
H	34.15101051973148	-22.42347712406486	10.61046874307694
H	32.62354881679320	-22.79297503514983	9.80306252424571
H	33.82179287361291	-21.77597648131009	8.99929920010737
H	37.06898169033992	-24.54974911932775	10.75952747790736
H	35.79031980283563	-25.52262915803458	11.48882806060070
H	39.77683039896282	-29.30623918487514	8.69381311165505
H	39.39657955889385	-27.66391525461117	9.22249181544932
H	38.38227889012586	-29.01298915595725	9.73803337232200
H	38.84869740111754	-30.87513726064703	5.60018880714278
H	39.80162776836033	-29.49309979480598	5.05454844838452
H	40.02504472201426	-30.13096105925032	6.68708826340089
H	35.64808438828923	-23.76217822618706	11.45494204943508
H	39.62096833064969	-23.15023863750592	3.72352609110671
H	38.69855014903143	-21.84310080880500	4.48699957578282
H	39.45718598873145	-23.09248132285981	5.48309636072616
H	33.31046924797562	-31.89987515006026	4.44320178077100
H	33.77716859675373	-33.23858203991217	5.50706522736046
H	32.63046255712730	-32.01727227819042	6.07996066015755
H	34.87607304191843	-31.57407485871574	7.06966279743790

H	35.59956131969187	-31.52465256929685	5.44381804942282
H	32.11877842848026	-26.35803440070281	7.3388557793644
H	31.44367358255339	-27.98383407052007	7.10764165997704
H	32.47950150353616	-27.68015431931525	8.47426148110156
H	36.89556299004960	-23.19280680140233	2.58738504615222
H	37.53787387926120	-24.96790484156689	6.34035483041158
H	34.98010790137413	-24.82522655860489	3.03169903103697
H	31.98381451674434	-26.88292876860477	2.18804864482468
H	37.07398458931072	-26.75680285739499	9.57491050353342
H	37.55150389651813	-29.50956835371629	3.84442424868729
H	32.48695820055104	-23.00373127909085	7.22594473176790

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B3LYP Scan/Melmid IPC Model/RKS/350 degrees Constrained Optimization

C	38.93280918291825	-22.95224707407194	4.50161672781795
C	37.69426298552334	-23.78637898826299	4.47438464808335
C	37.16193434987591	-24.68103636053434	5.36867423402574
N	36.79912520174623	-23.78257429477950	3.41362597586784
C	35.79262869469289	-24.65219028136311	3.70559578059919
N	35.98660265312406	-25.20928371119737	4.87984264243616
C	30.28452674319536	-24.83060916620583	2.77813113562927
C	36.00485211452390	-24.59859198487191	10.88706375631725
C	39.29493335324977	-29.88552069700861	5.94005624693553
C	33.31298575895663	-28.78055402653246	0.76955150409586
N	33.11790830465748	-25.57820028281162	5.13021477353825
N	34.74452485240373	-25.52396087203068	7.47173821231279
N	34.71035927764503	-27.67626836593825	4.07742964839646
C	32.63161428932546	-26.83960236970251	3.09073667516426
C	33.02419686166728	-23.88175491592284	6.89347165040802
C	36.52328892822497	-26.70157538582052	8.67208185240912
C	36.84606605788401	-28.83857012444330	4.35339831729569
C	30.64925660778223	-22.75101086531608	5.25980605443146
C	33.73878103614323	-22.62271660475704	9.63602631962689
C	38.97189384279928	-28.58819587741531	8.91061225078159
C	36.23636420639094	-29.98500452250784	1.53717421113197
C	32.36278926485773	-25.83381566805373	4.01601257879069
C	34.00691940327695	-24.40066618889546	7.73175341356245
C	36.91828586664603	-27.56202602274484	7.65086387294756
C	35.70276889050149	-28.50632213803776	3.63413985652630
C	31.30412659987684	-24.84384769431423	3.87860434271335
C	34.35111255424049	-23.85450413879461	9.03673155336594
C	38.09997795327063	-28.41195297009972	7.70247960445633
C	35.36805705240938	-29.04735489776111	2.32441918138508
C	31.45695280118721	-23.96934998810575	4.92177970644962
C	35.30128527339938	-24.68674336107578	9.56505415401353
C	38.23296569898449	-28.95914034502508	6.45465140818527
C	34.13759390168692	-28.54046744119101	1.99973325190740
C	32.58776928791142	-24.45194108734357	5.70036474230645
C	35.54502852014256	-25.71677103128839	8.56567723685470
C	37.10907460939210	-28.46889011432431	5.66842371390314
C	33.75479686572500	-27.66375521716759	3.09765178643800
N	36.32821743686145	-27.63331500672877	6.41778958626376
Fe	34.63450523037979	-26.70792531354353	5.84154833878190
C	34.66599924812839	-31.35248236676102	6.01536613981576
C	33.62882789817210	-32.07100077683725	5.16596226081628
C	32.31370927432622	-27.39889694725121	7.43232829155712
C	33.51352333061941	-27.84879855200006	6.65270064217483
C	33.62135032096351	-29.35730428368235	6.76918925711609
O	32.94715046782920	-30.01530900205131	7.53992956192540
O	34.51509724312793	-29.92057078992930	5.93994150191105
H	29.86751192312390	-22.56735936850792	4.51631337459001
H	31.27425705079283	-21.84923869865053	5.30727745694648
H	30.15471805056512	-22.84882501346937	6.23554078193472
H	30.75047701467974	-24.72812366286171	1.78856061799508
H	29.69752046580933	-25.75857685093268	2.75929781741998
H	29.57915739134596	-24.00180914504075	2.89360696846056
H	33.08815845185039	-27.84494235052972	0.23999134055543
H	33.82951781923995	-29.43875891920322	0.06403464060913

H	32.34977069451404	-29.24962740140669	1.01089572555105
H	35.79988393741070	-30.20891476233527	0.55852021748398
H	37.23546384411048	-29.56422278866420	1.36181128453153
H	36.38032156906098	-30.94218597702390	2.05638485304525
H	34.18983415753659	-22.38270809834568	10.60399905960667
H	32.65903447606736	-22.74265584809972	9.79859106674981
H	33.86939149175987	-21.74689982552444	8.98642046938033
H	37.09348843814652	-24.52037731614002	10.76381509605380
H	35.81704523209063	-25.48536175860740	11.50730034693238
H	39.79822187998641	-29.27814256058276	8.71324443977596
H	39.41139719180702	-27.63672949046849	9.24002917321339
H	38.40589760818634	-28.98981751840467	9.76174494986886
H	38.87644375296541	-30.84897300579883	5.61899057282145
H	39.81779965274277	-29.45909637800179	5.07333855035631
H	40.04900322681947	-30.09721121201143	6.70466410034726
H	35.67707635543960	-23.72508218568118	11.45942093919248
H	39.61557027303233	-23.19820813713096	3.67690551638471
H	38.71130795739408	-21.87811378763609	4.43979969853325
H	39.47200937379795	-23.12489656500578	5.43765696009520
H	33.65302848058311	-31.70253905883100	4.13716485061756
H	33.83366592963198	-33.14646440815665	5.15173226923629
H	32.62648019624899	-31.92013012375747	5.56987755908259
H	34.60348823741299	-31.66099114998792	7.06016823190827
H	35.67664367032816	-31.53101602366602	5.64520823771614
H	32.15901036865544	-26.32687744804807	7.40706569841232
H	31.40856602173740	-27.90136386160107	7.06643778879652
H	32.41222163977267	-27.72379506462995	8.47551119820903
H	36.87866858584645	-23.23232986972842	2.57063414633596
H	37.54868227606026	-24.97918023263126	6.33204055863926
H	34.95739682673090	-24.84768655926190	3.04930593586410
H	31.95273020056160	-26.93271312570889	2.24869098211124
H	37.08498151926478	-26.74258340830620	9.5999829923968
H	37.56088583166040	-29.49864222974180	3.87144915346404
H	32.51128762358187	-22.98616678837627	7.22949417045905

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B3LYP Scan/Melmid IPC Model/Triplet/0 degrees Constrained Optimization

C	38.98632814662176	-22.84041323686434	4.90417711581312
C	37.80307283539847	-23.73580840549360	4.73293425961336
C	37.14678278013869	-24.57374856591866	5.59777903397633
N	37.11519014807356	-23.86693354921394	3.53341068338421
C	36.10084533330094	-24.75350742784571	3.71883419956089
N	36.09672241985143	-25.19658982606587	4.95708130753871
C	30.51604497131883	-24.87431044240054	2.43629729805300
C	35.56083937682404	-24.61272286360721	10.97580821538051
C	39.25505683295712	-29.89880637575813	6.29801380428997
C	33.70491406408605	-28.83971743169547	0.68197150347161
N	33.20535114700562	-25.57698083881461	4.96211882579968
N	34.64729230936185	-25.51568859338934	7.44755700725919
N	34.85657781866365	-27.66947423486736	4.06139391026638
C	32.86272369527104	-26.84974627871161	2.90242428544462
C	32.95324187124416	-23.89700819615425	6.73001167258002
C	36.31216030720015	-26.68672225012513	8.80073179648185
C	36.95060856610903	-28.84899624891602	4.52802263919546
C	30.67162718168636	-22.80766018717230	4.94825374513068
C	33.40388052339872	-22.64779923901112	9.52936249710017
C	38.72603473622616	-28.57818682696987	9.22664788403764
C	36.55089257577232	-30.04862274577528	1.70297071819709
C	32.52675712774479	-25.84180925339444	3.80209975227569
C	33.87080843734203	-24.40512307315533	7.64493476262231
C	36.78522717581959	-27.54018016019329	7.81087217276948
C	35.86971828352139	-28.52107398355890	3.71713830716956
C	31.46256341997919	-24.87377105096648	3.60069993829183
C	34.08505181520533	-23.86618908243250	8.97966471214004
C	37.94830532834753	-28.39947804809629	7.95619988557200
C	35.63337741611265	-29.08545254811402	2.39735894286643
C	31.53059479595810	-24.00232162628891	4.65680256472392
C	34.99004760222046	-24.69385056984256	9.59082818676042

C	38.17017242922187	-28.95481773576475	6.72415901721133
C	34.43638267478398	-28.57622362453504	1.96527935802653
C	32.61500384915190	-24.46804168582933	5.50643803274022
C	35.34079021581326	-25.70843212627096	8.61170294596670
C	37.11652420829432	-28.45950254773797	5.85192864028321
C	33.97741148985732	-27.67436746541939	3.00835565798070
N	36.29400194371635	-27.60509008576269	6.53273082793751
Fe	34.69191107648027	-26.66647991962546	5.78720756059312
C	34.57054456458909	-31.33099771479364	6.08408048971021
C	33.80588420167195	-31.96301414596278	4.92858991289828
C	32.08048247042111	-27.31482212905584	7.14653333231597
C	33.34657733113478	-27.87686188888189	6.56228252554727
C	33.37761186351519	-29.33190194662690	6.58682324811481
O	32.47624669948417	-30.03802936297263	7.03259524377114
O	34.50511192352571	-29.89935845462015	6.06057462286415
H	29.94029692565722	-22.63368905495446	4.15288820386478
H	31.26903089799528	-21.89209640425936	5.05087849338718
H	30.11164466141955	-22.93154184943073	5.88474988128841
H	31.04570030993057	-24.78120766379965	1.47856594556285
H	29.93209602360291	-25.80304660169126	2.39007973296669
H	29.80467692462602	-24.04502643335324	2.49699897288104
H	33.50752102455011	-27.91301290772347	0.12678074543943
H	34.27726592368165	-29.49923104295904	0.02226504314694
H	32.73352574137417	-29.31896280833200	0.86143882470040
H	36.19537266805908	-30.28468841086689	0.69529326783639
H	37.56691561222090	-29.64333983414780	1.60651691139574
H	36.63485954881710	-30.99647934529031	2.25091777857457
H	33.76109607727329	-22.40997780189311	10.53606165197608
H	32.31594833972964	-22.78418698034023	9.59191752227122
H	33.58130044655690	-21.76582562634042	8.89974825919071
H	36.65366090042312	-24.50345052338497	10.96026455694268
H	35.33758911585136	-25.51576378710444	11.55911888197765
H	39.57021297216132	-29.26019633491316	9.08649274334405
H	39.13129285683295	-27.62615374952731	9.59531490968801
H	38.10040595808347	-28.99246914901981	10.02842858639713
H	38.84839350497902	-30.86483839962529	5.97043516386426
H	39.83504322941832	-29.49347837545327	5.45815506302722
H	39.95701521408376	-30.10084145592760	7.11303037058683
H	35.15480158859414	-23.75947318707718	11.52757851333136
H	39.81249850560388	-23.11423188219771	4.23443718047124
H	38.73931733250250	-21.78725607757451	4.71381809326024
H	39.35608303199536	-22.91245329516321	5.93103974004731
H	34.14890304279282	-31.55947644442993	3.97196082130187
H	33.95754658265072	-33.04801284520700	4.92068505705066
H	32.73771242363986	-31.76626210318705	5.02741522150004
H	34.19154257309343	-31.69552442184030	7.04139811255423
H	35.63823491260509	-31.55337659517700	6.01578843375913
H	32.24612980361049	-26.38890590851264	7.69615285313542
H	31.35567997628983	-27.08006057924398	6.35353535556666
H	31.60290708499528	-28.04305422272516	7.80507185019301
H	37.32954157026270	-23.38794092444025	2.67037810959329
H	37.35974117511132	-24.76904042577204	6.63826541134799
H	35.40459163185923	-25.04500890395112	2.94633360357265
H	32.24520364862757	-26.95487419752589	2.01644740034837
H	36.78994151202266	-26.73627916145723	9.77370323672130
H	37.68999619542613	-29.52876434981257	4.11679655572321
H	32.40028623156772	-23.01220203269461	7.02843361649408

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B3LYP Scan/Melmid IPC Model/Triplet/10 degrees Constrained Optimization

C	38.99990394856039	-22.86682853770373	4.89908114040007
C	37.80911087371315	-23.75261178656371	4.73018287353146
C	37.14727673524830	-24.58427050378696	5.59678470128870
N	37.11921157402003	-23.88025780561308	3.53139969541327
C	36.09832680401056	-24.75883870378060	3.71897844694671
N	36.09208762848881	-25.20019278941144	4.95784985433862
C	30.51025777777735	-24.86999354267731	2.43903328314912
C	35.56078909920279	-24.60882078559000	10.97598942848877

C	39.23320007437172	-29.91931629579587	6.30633989237470
C	33.70335344376523	-28.82602168110270	0.67774891123352
N	33.19743991161116	-25.57606543311068	4.96633310142216
N	34.64449611086952	-25.51301968232483	7.44883162144475
N	34.84700579709793	-27.67228747545866	4.06550869786303
C	32.85669133211099	-26.84539629251300	2.90433346697795
C	32.94744916881329	-23.89587348798087	6.73374519012535
C	36.30719983609178	-26.68670653698980	8.80276124980875
C	36.93965285089106	-28.85429039218197	4.53231600685486
C	30.66408515038101	-22.80623720489343	4.95353761873112
C	33.40407597866603	-22.64340325272617	9.52993538111055
C	38.70739700188038	-28.59495187962465	9.23397315648606
C	36.54468863044183	-30.04207336902677	1.69954851663711
C	32.51937748180597	-25.83971373053615	3.80582257295298
C	33.86803717960547	-24.40224277047277	7.64647483318277
C	36.77750338227234	-27.54255341553986	7.81369626864444
C	35.86024839174357	-28.52375645393565	3.72022414458408
C	31.45522410073935	-24.87133039838048	3.60466997440238
C	34.08401050354589	-23.86260415900051	8.98042178825856
C	37.93474014600365	-28.40952517617532	7.96144177007864
C	35.62680830609342	-29.08145888629374	2.39710584707100
C	31.52246698835815	-24.00123662859302	4.66176342868046
C	34.98915713864345	-24.69049596777931	9.59137529468422
C	38.15542590456581	-28.96609201620233	6.72991190868830
C	34.43163318027793	-28.56845223424800	1.96401337754767
C	32.60684855129995	-24.46778975774614	5.51132408473092
C	35.33857431425619	-25.70577899957805	8.61273912803078
C	37.10673868109960	-28.46350239336320	5.85563828094605
C	33.97060814234592	-27.67118719042918	3.00976236234884
N	36.28871130900054	-27.60388539782746	6.53476934821822
Fe	34.68600526819132	-26.66506189427794	5.79042222732812
C	34.56715833636451	-31.33473231732247	6.12608845468759
C	33.92411131771113	-31.90701708537236	4.86955857688023
C	32.08976592480171	-27.31729711137958	7.18492309653964
C	33.33742088474322	-27.87648369580227	6.55887962975183
C	33.34994002159805	-29.33136559857388	6.54050933017903
O	32.38077745299521	-30.03292050045562	6.82006395832340
O	34.53241997385016	-29.90142196660485	6.15768709629345
H	29.93316916968662	-22.63142639141377	4.15796468006518
H	31.26200622392917	-21.89105955986781	5.05679284830486
H	30.10368032384520	-22.93023598241264	5.88976197333969
H	31.04150857097530	-24.77757505672226	1.48210305663674
H	29.92477064488115	-25.79769316414743	2.39180242386130
H	29.80035675265865	-24.03937730262762	2.49887599648690
H	33.49842669795630	-27.89586336888367	0.13127708941447
H	34.28165053735908	-29.47452359003231	0.01231058013912
H	32.73603642896223	-29.31533966033877	0.85215696475031
H	36.19878998867217	-30.26066082096115	0.68460163710820
H	37.56479374382846	-29.64349881893784	1.62076582078945
H	36.61485595186202	-30.99885313148382	2.23392964579719
H	33.76154513190003	-22.40567421749143	10.53656318427767
H	32.31601386436915	-22.77873409710926	9.59254996836737
H	33.58228193461034	-21.76177559371087	8.90006331097433
H	36.65369394207359	-24.50067762488508	10.95983270232194
H	35.33692709451361	-25.51116734905204	11.56017647699429
H	39.54937317028494	-29.27988011805558	9.09475469994544
H	39.11510177099489	-27.64565092201272	9.60694628360156
H	38.07735784343237	-29.00919025118617	10.03236628841531
H	38.81882829523072	-30.88218715266689	5.97908253422397
H	39.81795877263435	-29.51993515101312	5.46693850787192
H	39.93211444196464	-30.12642949163066	7.12270250363636
H	35.15580373614517	-23.75475694827670	11.52728403703438
H	39.82402163504826	-23.15003208390771	4.23071115541581
H	38.76216443686484	-21.81219795445438	4.70518157707700
H	39.36850240978017	-22.93877028105921	5.92637821013117
H	34.37250471181203	-31.47174781437315	3.97272609794913
H	34.06345231905147	-32.99327751841976	4.83406007939472
H	32.85428328713035	-31.69678564939195	4.86170567191478

H	34.07782286905315	-31.72823241500276	7.02011600488867
H	35.63159702538498	-31.57787516387268	6.16722759079510
H	32.28002755984553	-26.40782533109908	7.75381986044376
H	31.34947300815833	-27.05382413971464	6.41564268097045
H	31.61464176312372	-28.05567781340998	7.83439762145055
H	37.33656183089498	-23.40434846142095	2.66740971730765
H	37.35984235483607	-24.77998979512904	6.63725233201721
H	35.39947595061065	-25.04654643192175	2.94737836793387
H	32.24067925416951	-26.94792970018612	2.01701500398287
H	36.78373610222108	-26.73765063630673	9.77628224468312
H	37.67688996873139	-29.53692574758265	4.12200425580519
H	32.39468285558728	-23.01117020608131	7.03285299582053

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B3LYP Scan/Melmid IPC Model/Triplet/20 degrees Constrained Optimization

C	38.99974318043734	-22.87455357687209	4.88901379187638
C	37.80667838090481	-23.75857824957367	4.72690249985074
C	37.15446938685780	-24.59704006776277	5.59432658068058
N	37.10242285005793	-23.87548324086671	3.53544309106919
C	36.08297810472639	-24.75464260979358	3.72765961895194
N	36.09111113025372	-25.20656308289868	4.96282459855513
C	30.50402600460933	-24.87769000086702	2.44634079363216
C	35.58460299339653	-24.58677443577314	10.96767657500318
C	39.21619720119279	-29.94341170921972	6.32140510782893
C	33.71890968772497	-28.80560425081483	0.66949189802190
N	33.19414643029742	-25.57878118367838	4.97202940170560
N	34.64615857265488	-25.51182109515995	7.45160317034220
N	34.84400082160245	-27.67852698091085	4.07237288506724
C	32.85959603029904	-26.84274998606556	2.90594271527429
C	32.94288332856288	-23.89931717567079	6.73931356354838
C	36.31391751095270	-26.68024418360143	8.80469868248732
C	36.92943377592844	-28.87121584361902	4.54458955598271
C	30.64941353379029	-22.81912340799017	4.96584386298999
C	33.41609522584920	-22.63197339870338	9.52494740716223
C	38.70729399018737	-28.59488047189624	9.24123144545755
C	36.55183712824751	-30.03297099317582	1.69800721540643
C	32.51736492801201	-25.84199706318325	3.81082032373658
C	33.86981174369475	-24.40050109741800	7.64830272816730
C	36.77634238998670	-27.54514306375460	7.82007305779869
C	35.85665032960664	-28.53141631102230	3.72754937769111
C	31.44936420417066	-24.87717453340508	3.61160925194044
C	34.09328235906102	-23.85386829204880	8.97788048034560
C	37.93015664908573	-28.41648647976383	7.97042203914066
C	35.63081065296886	-29.07755842592692	2.39862787084208
C	31.51300255534114	-24.00949217623132	4.67068779546265
C	35.00315468009327	-24.67767763062149	9.58764752666794
C	38.14390903615632	-28.98301583540257	6.74249949439432
C	34.43975893041529	-28.55806875346843	1.96174965623494
C	32.59986777352267	-24.47361394801688	5.51883106110520
C	35.34663965136826	-25.69838042551117	8.61283915156401
C	37.09582468765863	-28.47980659670939	5.86760787567012
C	33.97372521561721	-27.66828867804010	3.01116200886125
N	36.28322040989476	-27.61253128399870	6.54313516113996
Fe	34.68407782474206	-26.66787781913031	5.79642215549122
C	34.49505151931584	-31.36418216179942	6.15996445013409
C	34.01516757343725	-31.87932048730305	4.80967490015432
C	32.10405148308083	-27.31939250784394	7.23112827497355
C	33.32627811666060	-27.87813002461372	6.55419822711194
C	33.29931303163085	-29.32965867052017	6.46573675902035
O	32.27397863028801	-29.99934805915669	6.55836405244306
O	34.50570314334279	-29.93089674402271	6.23559248247195
H	29.91664338175124	-22.64636981992099	4.17152388945773
H	31.24312194226582	-21.90128295478675	5.07001940855652
H	30.09081375147854	-22.94749189314448	5.90254930145525
H	31.03478705157682	-24.78315683460424	1.48933355180114
H	29.92125132452647	-25.80705482604031	2.39884653284311
H	29.79187688165508	-24.04905045421853	2.50696162520304
H	33.51151548662514	-27.87084089829133	0.13199220997064

H	34.30365535514741	-29.44407894554612	-0.00000507380822
H	32.75351648512295	-29.30197347979892	0.83453552478681
H	36.21715957444654	-30.23402213082596	0.67571555627339
H	37.57481737610225	-29.63865637101249	1.63794788257577
H	36.61070635352283	-30.99868799945042	2.21765990891617
H	33.77857632270111	-22.38938925859525	10.52862087909894
H	32.32835776808576	-22.76695516524519	9.59360170167582
H	33.59116555478035	-21.75340733130448	8.88994892097922
H	36.67713336214152	-24.47645667574804	10.94284335494032
H	35.36700769492226	-25.48602284537890	11.55895780941309
H	39.54703714948368	-29.28283239780724	9.10344743214449
H	39.11901401793697	-27.64396354503231	9.60566404464208
H	38.07958257396870	-29.00174078323226	10.04523139852386
H	38.79585923771720	-30.90342346386992	5.99360917749192
H	39.80529310567140	-29.54830212847963	5.48293567024647
H	39.91225966300144	-30.15468783197587	7.13915070273209
H	35.18190680521062	-23.73023541158785	11.51680583582382
H	39.81576841397109	-23.15224870310843	4.20850893694111
H	38.75992036021115	-21.81831458434197	4.70671081852888
H	39.38054650565640	-22.95504721685849	5.91121143425176
H	34.60730429331272	-31.45097804044800	3.99737722663370
H	34.10813161941768	-32.97031201275972	4.76764646275560
H	32.96876167140677	-31.61552968240948	4.65563987515085
H	33.87018128592678	-31.76181004979176	6.96313712041124
H	35.533464447670614	-31.64997449574610	6.34365699740435
H	32.33260442119354	-26.44534924738047	7.84027742652085
H	31.35522646549916	-26.99849907849105	6.49280908738253
H	31.61937745207817	-28.07471333017556	7.85439936912021
H	37.30974469125645	-23.39219942322613	2.67307998759520
H	37.37922726668371	-24.80152673189465	6.63054571481215
H	35.37441634475906	-25.03471361830010	2.96214530293926
H	32.24665875401721	-26.94218416538833	2.01617494176066
H	36.79508604030445	-26.72541202022330	9.77622835958920
H	37.66385766637552	-29.55815917087207	4.13650921667110
H	32.38905824869605	-23.01550806185999	7.03911755233004

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B3LYP Scan/Melmid IPC Model/Triplet/30 degrees Constrained Optimization

C	39.02868493239535	-22.92117676980908	4.85261890669745
C	37.81770123827604	-23.78275675898108	4.70349263772574
C	37.16765387200318	-24.62112273206921	5.57267050207646
N	37.09004866981319	-23.87348737764920	3.52377845423444
C	36.05973165908436	-24.73789437847769	3.72425759491884
N	36.08298685219629	-25.20508958987168	4.95353507629292
C	30.51346290480718	-24.84489670091308	2.41887956313761
C	35.55676436120261	-24.60577803965792	10.96598581032498
C	39.19646646309789	-29.95067784225223	6.30765910298682
C	33.71438659982132	-28.78343971475488	0.64840958653911
N	33.18530312389052	-25.56656784119861	4.95854771946778
N	34.62987070837366	-25.51378292710670	7.44258943944763
N	34.83012515085896	-27.67335629633745	4.06058182856168
C	32.85708133513124	-26.82106310569465	2.88588444253105
C	32.92161795383597	-23.90259036129283	6.7369711730948
C	36.30068628286598	-26.68267022612913	8.79342345633107
C	36.91159812586749	-28.87321607543819	4.53318956415242
C	30.64651666131111	-22.80052450730480	4.95085335010541
C	33.37291239709567	-22.65997284586491	9.53463988603817
C	38.69256488858887	-28.60126050839797	9.22837313884668
C	36.53576682318409	-30.02796696641885	1.68406486152343
C	32.51466741486327	-25.82211203946720	3.79230424998718
C	33.84463079974682	-24.41004525741488	7.64575217288067
C	36.76455709616482	-27.54529745445658	7.807703988699426
C	35.84031300977486	-28.52969446857373	3.71579346736323
C	31.45082487242379	-24.85290929896302	3.59049392722278
C	34.06098929105748	-23.87202729686727	8.97948279745621
C	37.91600623621410	-28.41988013779831	7.95768504208583
C	35.61680688112399	-29.07051842070372	2.38459658766526
C	31.50873656182689	-23.99172083959947	4.65492305872513

C	34.97713563460354	-24.69244393971509	9.58491728033995
C	38.12767773505966	-28.98681396502441	6.72966258599640
C	34.43053637208661	-28.54295164871739	1.94462903372995
C	32.58925430995964	-24.46352485699440	5.50764173752532
C	35.33007722954574	-25.70346231874885	8.60384662559947
C	37.08046925944597	-28.48056869816564	5.85542007298290
C	33.96464165269855	-27.65465823232864	2.99530343581761
N	36.27112548819589	-27.61051419355894	6.53088601683223
Fe	34.67218993285620	-26.66291771443832	5.78740561931297
C	34.49551775066746	-31.36316838261945	6.24389515613834
C	34.15346064575765	-31.88164222874783	4.85403401177679
C	32.15594735533197	-27.31317981281887	7.33863780315626
C	33.31114164095872	-27.87212132223422	6.55127713597794
C	33.28383498170472	-29.32526945654508	6.45692397027654
O	32.25299707759178	-29.99140627489251	6.46220650670664
O	34.50252640614213	-29.92852955360842	6.31504005760468
H	29.91559193081794	-22.62504846312489	4.15541737552242
H	31.24145764084076	-21.88380788686639	5.05817655151147
H	30.08569176724120	-22.92988454848489	5.88607774987501
H	31.05091317263812	-24.74845800430767	1.46580598409089
H	29.92761988655010	-25.77193125519320	2.36375268623930
H	29.80403707432008	-24.01381387003971	2.47811537087824
H	33.47937600754101	-27.84376254820113	0.13172206267456
H	34.31609788238683	-29.39023387996188	-0.03548975968960
H	32.76392224666005	-29.31109976694157	0.80372898644250
H	36.21037421442965	-30.21474729223540	0.65603987732292
H	37.56328705244622	-29.64370655144789	1.63948306130067
H	36.57898921870001	-31.00008833416470	2.19347236213712
H	33.73100107701727	-22.42252000174870	10.54110770335867
H	32.28617682217374	-22.80444458446992	9.59941240473447
H	33.54237420181747	-21.77488951649351	8.90724183396687
H	36.64825803250078	-24.48542049811644	10.94247328781466
H	35.34710279616696	-25.51094236458038	11.55106273830529
H	39.53409505218267	-29.28663384318732	9.08858054879001
H	39.10156146165517	-27.65076250066051	9.59685078492072
H	38.06521344633025	-29.01276456374787	10.03032846080265
H	38.77301454764023	-30.91101300837072	5.98477384580070
H	39.78286463744550	-29.55961282965038	5.46543029954087
H	39.89544527120041	-30.16049727717568	7.12330410308389
H	35.14607756138052	-23.75666492426529	11.52066271918385
H	39.82809713258922	-23.20775208678000	4.15621541706915
H	38.80464824848338	-21.85945116925602	4.68261250941772
H	39.42528804790332	-23.01651958761813	5.86751708517190
H	34.82684592120734	-31.45776267166090	4.10552645210947
H	34.24530771043393	-32.97316418477057	4.82488757712263
H	33.12916888435878	-31.61543550843333	4.59196301412773
H	33.79173241147301	-31.75540189243241	6.98150428501318
H	35.50936095270085	-31.65011037813684	6.53275374721074
H	32.50745194765675	-26.77610940240365	8.22638831314563
H	31.56735524567290	-26.59272928248273	6.76039970036465
H	31.48391523849948	-28.11177848288133	7.65930379790700
H	37.28955158391717	-23.38281378538909	2.66374990736701
H	37.40818284156972	-24.84303005860858	6.60174211943565
H	35.33264145798443	-24.99726518208884	2.96889789049464
H	32.24861919746122	-26.91406546057539	1.99239860613319
H	36.78007930921729	-26.72998241387705	9.76572857803417
H	37.64360439068955	-29.56279269991277	4.12515786072604
H	32.36442682159513	-23.02275415363398	7.04211742113726

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B3LYP Scan/Melmid IPC Model/Triplet/40 degrees Constrained Optimization

C	39.02687107756588	-22.90837482816883	4.85680403024886
C	37.81629206878893	-23.76939248744196	4.70137775636813
C	37.16540400836735	-24.61236468247341	5.56537514862953
N	37.09048120112678	-23.85461862895529	3.52006217450276
C	36.06016496432014	-24.72034993733469	3.71466411913428
N	36.08202073647532	-25.19374032389888	4.94159425280473
C	30.51505515242808	-24.80686287374920	2.40850967941004

C	35.55477252676148	-24.62073893885227	10.96032367580531
C	39.15464778984290	-29.99056087152797	6.29359743079195
C	33.69227855363855	-28.75904760327341	0.63072844912644
N	33.18232229658697	-25.54797995967707	4.94764436723240
N	34.62766743124099	-25.50879125983769	7.43188883363925
N	34.82167331831616	-27.65807395972928	4.04100642025517
C	32.85448619848071	-26.78982097382724	2.86732802812113
C	32.91574905635598	-23.89661050686064	6.73744351545329
C	36.29719234981485	-26.68656872763334	8.77681334754951
C	36.88975460369996	-28.87941565180261	4.51491481126567
C	30.64071592243543	-22.78424944434157	4.95818320625490
C	33.36590567575408	-22.67078464720258	9.54247717032778
C	38.66617709284241	-28.63279263749945	9.21274385382795
C	36.50093830426868	-30.03435499661050	1.66801987598509
C	32.51350313777014	-25.79477989472187	3.77857093969455
C	33.84023655705839	-24.40803633256892	7.64249517123751
C	36.75568762151837	-27.54965612358919	7.78914354830173
C	35.82253048259100	-28.52548696675689	3.69651786702315
C	31.45019023330381	-24.82384933550170	3.58176734326282
C	34.05642985637236	-23.87768014874878	8.97916869913362
C	37.89541872326751	-28.43905348044837	7.94039933934951
C	35.59310472139846	-29.06473433562519	2.36571603700043
C	31.50530986951876	-23.97146096838919	4.65325510281188
C	34.97479733223361	-24.69982742876197	9.57893402586661
C	38.10105076856836	-29.00904238679209	6.71282248483528
C	34.41289895644005	-28.52448578808425	1.92548906307410
C	32.58453343730582	-24.44963286735107	5.50418977803873
C	35.32867277971621	-25.70440999543178	8.591770670603645
C	37.06284503075236	-28.48751764332306	5.83695255281750
C	33.95626601903005	-27.63086185118477	2.97565885391658
N	36.26460688207865	-27.60651575353218	6.51099830976805
Fe	34.67138155872314	-26.64887202648467	5.76989950940880
C	34.48975408359658	-31.37573150472594	6.37075127126730
C	34.35161580371605	-31.90850191159062	4.95139155264074
C	32.17283204595248	-27.32953358803519	7.34363618695189
C	33.31288947730960	-27.86890742807618	6.51998617983438
C	33.28843659571619	-29.32122281885983	6.39763975885176
O	32.26076056991344	-29.96882095902665	6.23570413215916
O	34.50783397028116	-29.93940963521934	6.43147063912627
H	29.91790993879085	-22.59635573363122	4.15816558339822
H	31.23492014069972	-21.86961607435007	5.08521903523105
H	30.07040345074726	-22.92720299880839	5.88573246393017
H	31.05488078910650	-24.71054041248245	1.45679477201316
H	29.92401408124725	-25.73036352592550	2.34937512083765
H	29.81028610284587	-23.97189403916052	2.46902319515933
H	33.50262316329699	-27.82071190521139	0.09284736702650
H	34.26841979638301	-29.40690791932539	-0.03713867069316
H	32.71798312588189	-29.23875200126661	0.79262310517472
H	36.15596453283926	-30.24470141618141	0.65103439007635
H	37.52634181716218	-29.64842938789260	1.59452799203855
H	36.55716296594828	-30.99447661724689	2.19826933413227
H	33.72261614394387	-22.44014572216699	10.55101525331148
H	32.27931195532664	-22.81730018064068	9.60500059688623
H	33.53464103357432	-21.78083651525351	8.92178350199048
H	36.64546168975934	-24.49311427989258	10.93720466362932
H	35.35148042950235	-25.53212296391481	11.53793637590811
H	39.50107483802468	-29.32628417192224	9.07324246592047
H	39.08389558160241	-27.68785121749990	9.58566458656537
H	38.03221055042270	-29.04051552869591	10.01145074047195
H	38.71573567626394	-30.94478231382816	5.97332537469843
H	39.74791240467381	-29.61169845897382	5.45061385595885
H	39.84970294809636	-30.20943779054814	7.11021846857835
H	35.13886011211673	-23.77901570493148	11.52234298631799
H	39.82945171319170	-23.19461150345931	4.16391655880606
H	38.80393524322368	-21.84645097282249	4.68669029869359
H	39.41863639736103	-23.00475733753337	5.87347901761459
H	35.14673326439299	-31.51882374035559	4.31205442831123
H	34.41314038475093	-33.00251686623429	4.95295825694311

H	33.38982517622591	-31.61804196236702	4.52874680947699
H	33.67744923462436	-31.74938097453140	6.99813862933981
H	35.44404310075461	-31.67330391475085	6.81145330306110
H	32.54142924744139	-26.84138567683678	8.25311407497350
H	31.58875869807413	-26.57304661549156	6.80831749238579
H	31.48968061595173	-28.13105633951341	7.63499915872201
H	37.29102301046500	-23.35959709702201	2.66277769550601
H	37.40432220213696	-24.83959704293179	6.59364666983026
H	35.33412758209553	-24.97629118167854	2.95711086852204
H	32.24678082511365	-26.87655788194981	1.97266416455856
H	36.77591030500150	-26.73969289407179	9.74916171601900
H	37.61468126000681	-29.57672345836223	4.10732300473967
H	32.35691861268759	-23.01991863980939	7.04860982479150

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B3LYP Scan/Melmid IPC Model/Triplet/50 degrees Constrained Optimization

C	39.04874139245594	-22.94701798174316	4.82002146065318
C	37.82075878368012	-23.78596572919958	4.68185023711636
C	37.17921322058152	-24.63575205922893	5.54644451523786
N	37.06265378473493	-23.83607891193374	3.51897838467942
C	36.02407669671324	-24.68927686264412	3.72395938207329
N	36.07062843004896	-25.18746518154519	4.94033923606167
C	30.50719555700701	-24.78479417597933	2.40277073804847
C	35.55775012222096	-24.60569654835636	10.95098801009468
C	39.12935780292935	-29.99929289180885	6.29527683679824
C	33.68748748495671	-28.73412420535121	0.61722177170047
N	33.16581386652130	-25.53815508188643	4.94799224197397
N	34.60497747470654	-25.50988237444780	7.43278255051842
N	34.80865498626204	-27.64870387176692	4.03530129054804
C	32.84666043405394	-26.76864558437536	2.86024930700074
C	32.90362546826144	-23.88614347590229	6.73702882946196
C	36.27883416387508	-26.68592506112446	8.77488949949504
C	36.86718477755915	-28.88347817738092	4.51481791343996
C	30.63044509084059	-22.76845859920315	4.95778456313736
C	33.37351231377805	-22.65121702401694	9.53368905694391
C	38.64794211848457	-28.63239324843646	9.21123915003322
C	36.47302463613820	-30.03645575740619	1.66227504957932
C	32.50127064244940	-25.77938151116529	3.77531926836828
C	33.82624713491359	-24.40231302299146	7.64172109823779
C	36.73576831499964	-27.55122904858553	7.78796550673817
C	35.80496805132170	-28.52230823269793	3.69236697085004
C	31.43986028797117	-24.80569153393090	3.57782948303206
C	34.05245019295175	-23.86643246516277	8.97416143446037
C	37.87497262758930	-28.44142004139692	7.93976072449989
C	35.57715471076641	-29.05539112304461	2.35937953424971
C	31.49287287185557	-23.95690354259427	4.65169943032775
C	34.96898549007329	-24.69065667780184	9.57362924560843
C	38.07811998816478	-29.01474741806657	6.71339545476879
C	34.40273381388333	-28.50432648192973	1.91586376996622
C	32.56916523765860	-24.43962217159126	5.50445390280856
C	35.31139764398826	-25.70285534106738	8.59042523982779
C	37.03985390718816	-28.49297761662578	5.83745534911407
C	33.94668745758908	-27.61293949146707	2.96759895566761
N	36.24382043059852	-27.60929936484864	6.51063723516350
Fe	34.65625203347658	-26.64257942137307	5.76713818135358
C	34.44918548675717	-31.40198477636732	6.42441495398066
C	34.54444085693552	-31.92272782910507	4.99774036479470
C	32.21149549589293	-27.37940323885055	7.40557283014198
C	33.29985793415155	-27.87922067676786	6.49353477484139
C	33.27122130477299	-29.33156345998804	6.32963269261697
O	32.26194100577956	-29.95927568362194	6.04028779103652
O	34.47084753038743	-29.96499280682310	6.49927298265452
H	29.90075283034799	-22.58491417553662	4.16301375775831
H	31.22535473896059	-21.85283210895063	5.07504102797115
H	30.06813539719207	-22.90669349764385	5.89088045898517
H	31.04884490736998	-24.68703183867907	1.45222585366664
H	29.91521904558481	-25.70751302462012	2.34062798937918
H	29.80340561716622	-23.94901236228005	2.46390018890178

H	33.41541843452926	-27.78979279112605	0.12862286761501
H	34.30674970260208	-29.29960497621039	-0.08640251881094
H	32.75784543591841	-29.30069676671665	0.76269224570809
H	36.20492968043803	-30.14139729978333	0.60614004953287
H	37.52506821804604	-29.72711774639730	1.70432499416954
H	36.41253526908834	-31.03642092992636	2.11318286201017
H	33.73917873682758	-22.41546981680129	10.53785065995506
H	32.28646956317415	-22.79026451683630	9.60539037712683
H	33.54325439245530	-21.76688070507844	8.90528797567300
H	36.64997645178201	-24.49398231445035	10.92032512516070
H	35.34475408037434	-25.50765756287067	11.53987166383012
H	39.48864935023620	-29.31832746141299	9.06914515326511
H	39.05764139410508	-27.68494654113992	9.58661551592896
H	38.01806423694546	-29.04776212511046	10.00929716961822
H	38.68975202476581	-30.96045298563823	5.99700879828863
H	39.70897231698365	-29.63206718414026	5.43790818070591
H	39.83694766426885	-30.20215304782037	7.10532472779302
H	35.15734149735990	-23.75195189704521	11.50613700632725
H	39.82595612967295	-23.23043027895005	4.09763780453255
H	38.83775643378211	-21.87839367262867	4.67897773686255
H	39.46877676259109	-23.07124383516088	5.82229027227945
H	35.44159505066693	-31.54148604377344	4.50534975285568
H	34.59020505320427	-33.01749995503999	5.00089944252316
H	33.67169473697104	-31.61574395479264	4.42024869906837
H	33.54050338202241	-31.77009813767348	6.90521872927035
H	35.31460901760320	-31.71274340865536	7.01426575202149
H	32.57552572651459	-27.29457286443565	8.44045937553360
H	31.83347449232577	-26.39552113826706	7.12511749277124
H	31.37075878044423	-28.08033804236864	7.40921317493673
H	37.24863180974355	-23.32743552443802	2.66637550212590
H	37.44180246528825	-24.88793674236999	6.56312166868437
H	35.27453195881659	-24.91922397370926	2.98108621364493
H	32.24185608460228	-26.85016196642102	1.96317165288286
H	36.76044468436407	-26.73663904361918	9.74596751482664
H	37.59051620733387	-29.58344366467184	4.10914067712431
H	32.35080816460471	-23.00531438820764	7.04715290779983

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B3LYP Scan/Melmid IPC Model/Triplet/60 degrees Constrained Optimization

C	38.98819365612102	-22.81004107229130	4.88133088042793
C	37.80157410974959	-23.70010678004178	4.70584756849796
C	37.14577149782721	-24.54419521323285	5.56495396435827
N	37.10833309186739	-23.81641268890444	3.50773444571438
C	36.09148774659653	-24.70072824870472	3.68763625385440
N	36.09068271061260	-25.15607600250263	4.92172591206660
C	30.53351711867761	-24.67417465686515	2.42294931992136
C	35.62416473710398	-24.65874764932830	10.95341902564356
C	39.09173037394128	-30.06438392608069	6.22163853962885
C	33.58899272387531	-28.70509917342588	0.61668077525460
N	33.18843837271393	-25.49337530822155	4.95265614250816
N	34.64484568147643	-25.49708756386094	7.42531597449934
N	34.80037265889646	-27.60711335472185	3.99875352665448
C	32.85059352613153	-26.68457903386642	2.84213286782973
C	32.91500594691420	-23.88543405644000	6.78346762319554
C	36.34598950527108	-26.68103485109424	8.72585930132015
C	36.80961163077789	-28.92601068206110	4.47395568271537
C	30.64281026325559	-22.73363988707643	5.03545636161365
C	33.38473505113556	-22.71405341972313	9.61045110806982
C	38.69792065942539	-28.65115102271715	9.12755567515587
C	36.33420388674550	-30.10780719925400	1.65286761580985
C	32.52262801318663	-25.70519213856209	3.77315702461259
C	33.85029205880200	-24.40944512211860	7.67050708619135
C	36.77980850737467	-27.54832723049584	7.73022676034551
C	35.75448360637370	-28.52933569841406	3.65947968016766
C	31.46298338513107	-24.72683960143322	3.59953909603849
C	34.08169892939748	-23.90089246719671	9.01359802613615
C	37.90420059224837	-28.45832274916271	7.86926710969986
C	35.48836020142155	-29.07571775903458	2.33860857179412

C	31.51114770657732	-23.90914158570547	4.69779069265760
C	35.02212014190039	-24.72006600046534	9.58066496141476
C	38.06819183033151	-29.05447330928749	6.64769369688691
C	34.33491119341682	-28.48162377878198	1.89855958320072
C	32.58685572408343	-24.41074910519932	5.53777296084390
C	35.36765825089569	-25.70518790766681	8.57046445773058
C	37.02314372149171	-28.52152216839343	5.78722488266009
C	33.92808878926279	-27.55713052306937	2.94159238606906
N	36.26399097803655	-27.60762022206098	6.46247346116944
Fe	34.68111192693080	-26.60036215387939	5.73644541080001
C	34.17252758905725	-31.49252778497815	6.66058940589759
C	35.01407029374524	-31.98493270717406	5.49360474655024
C	32.04906176093647	-27.43735861841482	7.02258861381851
C	33.38099931273886	-27.88473619608738	6.47955784652458
C	33.37446982081685	-29.31130455740258	6.10278880139378
O	32.64429166912809	-29.81528825839233	5.27112321060464
O	34.24839043585830	-30.06369931426750	6.83894772005549
H	29.91417208941764	-22.53102965458643	4.24438507717785
H	31.23292426188076	-21.81890109643519	5.18013443138870
H	30.07877875956487	-22.90095215257692	5.96276963842156
H	31.07794638777123	-24.54869539079941	1.47729482520539
H	29.94321673562679	-25.59566930929410	2.33252612859360
H	29.82816036557968	-23.84161696636880	2.50562858897750
H	33.39887793983802	-27.76374522742324	0.08448227807002
H	34.14653459187487	-29.35703689197508	-0.06297074154306
H	32.61359875529213	-29.17572154244730	0.79737554851756
H	35.98718332746713	-30.29531681109413	0.63201063443489
H	37.38544650347494	-29.79678447469297	1.59055772260536
H	36.31425308015979	-31.06777373525545	2.18594467010737
H	33.75457914129853	-22.49749605727954	10.61741748481548
H	32.30114272794267	-22.87576009615105	9.68725545382061
H	33.53177516146452	-21.81025612757745	9.00424631540491
H	36.71462541073119	-24.53319763167766	10.91451065060719
H	35.42828487853069	-25.57667196284481	11.52336424448933
H	39.52738383891091	-29.34844902244104	8.97507146665420
H	39.12620908934445	-27.70673168333646	9.48947025501669
H	38.07721625940518	-29.05371888381143	9.93926691395295
H	38.62921543837241	-31.01908896914383	5.93752364006873
H	39.66634191322490	-29.71648079983405	5.35287087935890
H	39.80667854725777	-30.27570556112165	7.02302969257973
H	35.21924641495675	-23.82284187728942	11.53207347990735
H	39.81120197477112	-23.07980908978498	4.20608712037985
H	38.74349093014249	-21.75442354698856	4.70180955952778
H	39.36123638525657	-22.89276671561959	5.90618423672229
H	36.06065610937681	-31.69831468288120	5.62009159797859
H	34.96115563865106	-33.07737411798471	5.42874869415084
H	34.64855857394389	-31.56421755421112	4.55603580530530
H	33.12702241233251	-31.77626648808614	6.52529293666419
H	34.53410468961074	-31.90160310832706	7.60665684823983
H	32.10740843469733	-26.46753158874801	7.51579160327899
H	31.28675811157931	-27.36283279993675	6.23177719337999
H	31.66323175346777	-28.15821348971074	7.75746401888572
H	37.32110713815051	-23.32956145314763	2.64872284844198
H	37.36142694068612	-24.75149454221898	6.60253275555296
H	35.39050832537395	-24.98213512120354	2.91565597295119
H	32.23762087255191	-26.74871286622403	1.94923383486801
H	36.84377036021664	-26.73863312153612	9.68837228243290
H	37.49561249821374	-29.66196256685431	4.06738228206074
H	32.35169282833063	-23.01979256602017	7.11653007254214

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B3LYP Scan/Melmid IPC Model/Triplet/70 degrees Constrained Optimization

C	38.97902279484710	-22.78318687235036	4.89116504291220
C	37.79741803999362	-23.67775271786195	4.70492818171848
C	37.13598278208212	-24.52302307960029	5.55849570250409
N	37.11690434800995	-23.79848743769099	3.49998578685970
C	36.10146641638340	-24.68632272559223	3.67092233987209
N	36.08967438270790	-25.13983291895518	4.90566802324179

C	30.54576469504747	-24.62758926874620	2.40270084781739
C	35.63233480111717	-24.68501123334330	10.94022419586950
C	39.07703231519971	-30.08292637493608	6.17948801259967
C	33.59534094318899	-28.64860731297928	0.56881383219561
N	33.18302559724168	-25.48388900589319	4.93855136398373
N	34.64288046933968	-25.50251333329643	7.40980361589662
N	34.80340901494348	-27.58335514742156	3.96252206716018
C	32.86205439503955	-26.64174102457054	2.80699371024379
C	32.89892301744096	-23.89883955790776	6.78858416456398
C	36.35493179756394	-26.68788481301810	8.69510963334410
C	36.79402447294903	-28.93114750742246	4.43866255423716
C	30.63029491833836	-22.73140944174379	5.04824593029406
C	33.37066597352118	-22.74788926408554	9.62380539393721
C	38.70018934143587	-28.66670057641124	9.08664022390565
C	36.31491021497096	-30.09298890526672	1.61142961768707
C	32.52628796829476	-25.67749504961867	3.75095132206140
C	33.84059142988167	-24.42405964013723	7.66820395774027
C	36.78457098030460	-27.55264330995577	7.69539224623164
C	35.74707182037938	-28.51600605188725	3.62288371841704
C	31.46582586770123	-24.69865681529453	3.58565639996716
C	34.07399829076493	-23.92456196219665	9.01435234071340
C	37.90395756049574	-28.46918415238657	7.83066924536399
C	35.48093776852220	-29.05158585496309	2.29744553086685
C	31.50372698370558	-23.89939408694751	4.69776461383121
C	35.02425605912844	-24.74022191761809	9.56986403024397
C	38.05943678576853	-29.06827277238267	6.60912780204743
C	34.33833333218929	-28.44018197688312	1.85477930257271
C	32.57549617386643	-24.41118340645824	5.53648987424994
C	35.37214179385414	-25.71488211761103	8.55005830006727
C	37.01474436560626	-28.52913855062836	5.75196394677877
C	33.93599437610980	-27.51894625599813	2.90261679002687
N	36.26466065333653	-27.60892970634991	6.42895723032967
Fe	34.68090310676663	-26.59361246293768	5.70841042308023
C	34.07542965619177	-31.51171920641141	6.79373553465196
C	35.08818114496149	-32.03278816990050	5.78616148769185
C	32.06395725639612	-27.47990227622988	7.00319577801305
C	33.40401527952692	-27.89550835765987	6.45708796399334
C	33.42696974671684	-29.32382252246265	6.07385135468630
O	32.84247740224552	-29.82591446355364	5.13523926690980
O	34.14457662356401	-30.08061128341620	6.95943929472680
H	29.90529271892833	-22.51911905627257	4.25635474286284
H	31.21708605818524	-21.81727180240923	5.20939826371295
H	30.06188747566650	-22.91386211786526	5.97002778353908
H	31.09773239648347	-24.48535499587014	1.46380476052564
H	29.95755779294028	-25.54822113134469	2.29185380309551
H	29.83855572184604	-23.79746889352299	2.49377160519730
H	33.40754858244141	-27.70142779978936	0.04626863132042
H	34.15367129218678	-29.29400748144844	-0.11643760760148
H	32.61903948016472	-29.12019661239075	0.74232915336642
H	35.97912128144123	-30.26080333229482	0.58338573846565
H	37.37330658981423	-29.80403492936254	1.56823434401121
H	36.26641672336014	-31.05882855668333	2.13206370964923
H	33.74297594683429	-22.53674047251801	10.63102889504465
H	32.28856920394529	-22.91806106647931	9.70353210026290
H	33.50870160446078	-21.83807351571323	9.02447321281548
H	36.72189869045739	-24.55325342420016	10.89712930456867
H	35.44410752560926	-25.60789169745881	11.50475631456259
H	39.52488069278257	-29.36916029836805	8.93198138877599
H	39.13514823031097	-27.72488297146743	9.44733005490723
H	38.07909308776466	-29.06544555205528	9.89994622970862
H	38.60992409189594	-31.03553591293567	5.89621471991701
H	39.65007839367102	-29.73663946850408	5.30905654024955
H	39.79367930234729	-30.29729391834562	6.97854722902729
H	35.22556615675342	-23.85528025920838	11.52647732962940
H	39.81044906311098	-23.05212463083221	4.22596332301139
H	38.73280222298537	-21.72891607718740	4.70590169575082
H	39.34079235995914	-22.86176068840123	5.92037767172437
H	36.09761574996961	-31.71069429852717	6.05278975386622

H	35.06837772376377	-33.12790809372249	5.76471600832747
H	34.85691850013592	-31.66159471909848	4.78700784950968
H	33.06096607563504	-31.78630098410398	6.49718572042325
H	34.27455000826686	-31.90707824507749	7.79226447929210
H	32.09750931220017	-26.50578673406552	7.49093316196316
H	31.29498228139440	-27.43062845339690	6.2160059902119
H	31.70361638934979	-28.20750807672499	7.74511243733589
H	37.33655848529600	-23.31204672412355	2.64247897488695
H	37.34145551651456	-24.72764549131065	6.59867194445007
H	35.40947753086572	-24.97142796834208	2.89220179202909
H	32.25486531179988	-26.69279673280048	1.90928473195005
H	36.85644924399688	-26.74929837721790	9.65546248345264
H	37.47063180562502	-29.67511619148896	4.03107837129236
H	32.33016720619899	-23.04052745108803	7.13126105799178

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B3LYP Scan/Melmid IPC Model/Triplet/80 degrees Constrained Optimization

C	38.99616088126064	-22.81811275541239	4.91843645418648
C	37.80667191097481	-23.69469590014144	4.69968653540020
C	37.12754415670162	-24.55268574089631	5.52627937251522
N	37.13619839324041	-23.77815595635464	3.48594579699825
C	36.10842796240618	-24.65714054447498	3.62607104056375
N	36.07997552589027	-25.14035728959878	4.84925689216635
C	30.56198408293601	-24.45687218729079	2.32995588896795
C	35.58084452111024	-24.86978110556965	10.89721155863567
C	38.97409729779947	-30.16760155150731	5.97832292967641
C	33.53382430113029	-28.48867707711336	0.40306003982896
N	33.17074030609941	-25.42759914494587	4.85358942335006
N	34.60921629855488	-25.56046164336357	7.33474519015208
N	34.75415365893065	-27.53956128426275	3.82741265073058
C	32.84451698614595	-26.51614677655566	2.68664072855161
C	32.88839641754911	-23.91163941387818	6.75730335210665
C	36.30852312519249	-26.79770922916104	8.58854497294220
C	36.70415402087841	-28.94941168921669	4.27964275919385
C	30.64326199733257	-22.65582869689804	5.04222578237662
C	33.34518861867763	-22.87095386439041	9.63112195556304
C	38.63996050807167	-28.80266135499813	8.91835867415678
C	36.19694328495482	-30.04381985550197	1.42772830987087
C	32.52066759525550	-25.57398705485187	3.65652523511334
C	33.81568680653289	-24.48169650442470	7.62335765899570
C	36.72972875508340	-27.63606738499704	7.56329534902848
C	35.66946639097581	-28.49290075449615	3.47028148237831
C	31.47277292641719	-24.57674398332312	3.51589074434716
C	34.04435506460724	-24.03099626278760	8.98622619310864
C	37.83651044226468	-28.57139554696026	7.67264605544965
C	35.39336602601297	-28.99148966304806	2.13282665208238
C	31.50901467300514	-23.81795191804918	4.65544990016271
C	34.98430671995946	-24.87269367998087	9.52073200886214
C	37.97558829376314	-29.14661592694119	6.43763170481053
C	34.27371498021033	-28.33335514151364	1.69826785960237
C	32.56940067542031	-24.37153600434774	5.48358582756363
C	35.33156510882082	-25.81488689745994	8.47180312633687
C	36.93577569395327	-28.57233435105384	5.59792693289821
C	33.89375262084531	-27.42443080447793	2.76558538152039
N	36.20460776910060	-27.65333724898852	6.29807854774774
Fe	34.64518980993649	-26.59235372541450	5.60496589925673
C	34.42260815675004	-31.39979091544745	6.48577535847501
C	35.33681228508726	-31.97462354016436	7.55099131032982
C	32.17320965620215	-27.49815098584191	7.17054294805350
C	33.30417248747455	-27.87902841235606	6.25834626548265
C	33.38775636718859	-29.31998302090715	5.96601866739118
O	32.70319690200091	-29.90463149799582	5.15018480539482
O	34.30336907286003	-29.98715524202162	6.73162063286946
H	29.92421891946416	-22.41093691069608	4.25438427715064
H	31.23629530481632	-21.75234618254219	5.23746918170873
H	30.06861595898719	-22.86553693968154	5.95430002560100
H	31.12160519326554	-24.28604009472050	1.40034628400548
H	29.96790691849216	-25.36867042841322	2.18336417972685

H	29.86039133832473	-23.62507077963622	2.44550809009801
H	33.37975587861367	-27.52407980752812	-0.09817405603258
H	34.07691186996495	-29.13503871046471	-0.29338776534414
H	32.54188261473778	-28.93334507752225	0.55821001058785
H	35.87113634889933	-30.16804415100206	0.39030156004458
H	37.26612773775452	-29.79508453438505	1.40825366896834
H	36.10298524656164	-31.02221632505919	1.91773518884437
H	33.71185124096790	-22.69672420869636	10.64739712153114
H	32.26159409533294	-23.03690658424827	9.69784602346618
H	33.49301532083583	-21.94212572143914	9.06429230463494
H	36.67406367135567	-24.76959416702708	10.86663851439241
H	35.36014087583871	-25.80028396309973	11.43708429345798
H	39.45117490630258	-29.51651115289924	8.74548139502541
H	39.09430207207289	-27.87401433393531	9.28914640779820
H	38.01962094660597	-29.20331064899165	9.73114912227561
H	38.48881356230717	-31.10715263577570	5.68147597519319
H	39.54406195192461	-29.81283737911040	5.10941139144207
H	39.69467682674599	-30.40820070391628	6.76623210549036
H	35.19341788380883	-24.04301489372443	11.50053079252452
H	39.83171457697422	-23.08179961754674	4.25631302724010
H	38.76367681594181	-21.75731963998615	4.75392432491721
H	39.34568990047912	-22.92328006954563	5.94948578874971
H	34.91580909035576	-31.81804649542786	8.54765702848863
H	35.46861250666083	-33.05090389158978	7.40017176795852
H	36.31845816459303	-31.49617518079242	7.52113104712707
H	34.82411868919749	-31.55253974769576	5.47877876936779
H	33.43014151862442	-31.85683568055807	6.51096876120098
H	31.81195136319542	-26.48438492577421	6.99125808965670
H	31.32250893099808	-28.18084153103166	7.04237143422669
H	32.46770082968852	-27.54649210065743	8.23185371405718
H	37.36946384696409	-23.27353561402310	2.64264861180267
H	37.32043244410835	-24.78557781913130	6.56292479257281
H	35.41994391252049	-24.91459050609071	2.83474804944026
H	32.24270515177883	-26.52799301499457	1.78384353452540
H	36.80867641843535	-26.89170120463654	9.54685089016212
H	37.36397989922274	-29.70082237809384	3.85839660305045
H	32.32728670571473	-23.06040081152747	7.12884451766969

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B3LYP Scan/Melmid IPC Model/Triplet/90 degrees Constrained Optimization

C	38.97853599547331	-22.75465050970853	4.95248841224060
C	37.80794566231854	-23.65429984655755	4.72566598969397
C	37.12259406592532	-24.50384184708086	5.55588752284430
N	37.16799500529546	-23.77641199427897	3.49886612984256
C	36.15150318661902	-24.66930273322150	3.63549724320815
N	36.10104711958122	-25.12426522158700	4.86857758421427
C	30.59507476195263	-24.51480675422893	2.33144868647374
C	35.58182259209288	-24.82474562506983	10.92325602460418
C	39.01491886855891	-30.15763820120636	6.06911822659242
C	33.63779488137018	-28.50765275151396	0.42711354988526
N	33.18947897011810	-25.46069520340896	4.87893799221027
N	34.63042018795589	-25.54058563346070	7.36048144771775
N	34.81076932452654	-27.54014814099198	3.86385680541594
C	32.88959158629155	-26.55666197941970	2.71123307984631
C	32.89096651730743	-23.92284608728210	6.76759176383961
C	36.32918080757291	-26.76295914509329	8.62852607570859
C	36.77793673349606	-28.92380051264828	4.32851868178822
C	30.65303494248745	-22.69511932274623	5.03056089660297
C	33.33145170626403	-22.85279966539555	9.63963672187176
C	38.65232321531218	-28.77416451620613	8.99531859450582
C	36.32234815526349	-30.00996402709513	1.47059485551893
C	32.54763412840543	-25.61665852228602	3.67759208831803
C	33.82398175194511	-24.47169876188926	7.64199706614178
C	36.75992347395728	-27.60953184496179	7.61376060917938
C	35.74683069207264	-28.47431204293767	3.51231660214324
C	31.49625430109405	-24.62694622536007	3.52572008187170
C	34.04410560939517	-24.00962505697230	9.00385100523776
C	37.86496338132152	-28.54418994550805	7.73908780530510

C	35.49297695973738	-28.97456952983826	2.17027788766099
C	31.52367082084461	-23.85923095823227	4.66060724696793
C	34.99077801879336	-24.83881534205351	9.54457794160621
C	38.01895045017560	-29.12569949833037	6.50794433040114
C	34.36395412788736	-28.34029361562322	1.72860370401943
C	32.58074203837390	-24.40013798879147	5.49848486679962
C	35.34950875910238	-25.78427438194944	8.50071975830098
C	36.99086777476285	-28.55447653516250	5.65282048905340
C	33.95690331047324	-27.44256477435346	2.79622682448433
N	36.24821464647726	-27.63616719808845	6.34218537716873
Fe	34.67493402590356	-26.59310912129096	5.63308576585807
C	33.89459187793926	-31.46728029950692	7.17454047401470
C	35.23298222648067	-31.99138871747056	6.67614810765921
C	32.03453640860178	-27.52321148380067	6.84939887646267
C	33.40830759208473	-27.90503698740222	6.37370436416176
C	33.54699178828118	-29.34956327970248	6.10626884252260
O	33.34078975216831	-29.93156166128274	5.06194931554492
O	33.87426037486368	-30.02799293920811	7.25398812783932
H	29.93439464920331	-22.46282408577377	4.23850021774755
H	31.24279676226083	-21.78726721472550	5.21485356309920
H	30.07766119284466	-22.89457174868065	5.94441954922020
H	31.16223312089439	-24.34190374746753	1.40680711804076
H	30.00760661920644	-25.43013620447099	2.18006778577575
H	29.88747490765530	-23.68705311396361	2.43912632462861
H	33.44424060242265	-27.54348484909412	-0.06090062451623
H	34.21203537572484	-29.11950775457647	-0.27568588697473
H	32.66536507448803	-28.99787816486343	0.56926622801288
H	36.02212070135595	-30.12278532508616	0.42404962768317
H	37.38945008888311	-29.75247971800643	1.47958199794151
H	36.22402962898920	-30.99520612539278	1.94583175373523
H	33.69373530049570	-22.66850326346787	10.65574281049458
H	32.24927136877008	-23.02870259074710	9.70473377257539
H	33.47155045249430	-21.92610401067700	9.06722297646627
H	36.67436808540706	-24.71631160560760	10.89674928379899
H	35.36592261358037	-25.75466177720781	11.46613273859884
H	39.46891417674644	-29.48410731886822	8.83201916596834
H	39.09730140687790	-27.84413267195724	9.37377372295532
H	38.02282317335792	-29.17877265602650	9.79910577482158
H	38.52596186768235	-31.10339966803462	5.79969879895022
H	39.58009742594346	-29.82566268457730	5.18829840579969
H	39.74006476263766	-30.37880198283069	6.85865467241789
H	35.18548903588790	-23.99838387451822	11.52135820172262
H	39.83202600127731	-23.01694214364509	4.31306468377949
H	38.73314371001894	-21.70084179238007	4.76351163909389
H	39.30767995125072	-22.83547230619640	5.99241032853571
H	36.05121124578467	-31.60994312487563	7.29231321134107
H	35.25021561688948	-33.08609826742869	6.71461899610683
H	35.40107115092273	-31.67896049029808	5.64457836256601
H	33.08266065655406	-31.80126931469211	6.52520700765581
H	33.69646698947408	-31.79968328120977	8.19605081430582
H	32.01505083500309	-26.54350585235153	7.32851302482409
H	31.30662798221977	-27.49574172253612	6.02248598942448
H	31.65905515688519	-28.25677088370550	7.57658886330818
H	37.41375869860980	-23.28828503461118	2.64944734571098
H	37.29496011165807	-24.70966737612518	6.60180757090733
H	35.48717638510743	-24.95713660979845	2.83399189681215
H	32.29396462237074	-26.57805608430336	1.80454311029823
H	36.82310959186306	-26.84960280665267	9.59084264432359
H	37.44747848510524	-29.66901074037509	3.91179648227370
H	32.31986282326990	-23.07300967498915	7.12704990642031

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B3LYP Scan/Melmid IPC Model/Triplet/100 degrees Constrained Optimization

C	38.96693141248248	-22.71214783193043	4.96809353532446
C	37.80254616275801	-23.61899260912665	4.73796557204605
C	37.13316933128005	-24.48892336666830	5.56003565612008
N	37.15196583130005	-23.72643967732419	3.51526797415854
C	36.14515627368828	-24.63085532550470	3.64631457570060

N	36.11081771320350	-25.10722568776113	4.87192571220041
C	30.58657531251167	-24.53773884024431	2.33535461136445
C	35.59696849201818	-24.82865752941342	10.91415282979212
C	39.03455093132158	-30.15344989511905	6.05596658406804
C	33.67107319109768	-28.48763244423947	0.40839079450510
N	33.19981170781946	-25.46450176631591	4.87063090798038
N	34.63884666938678	-25.54814741034881	7.35382008110509
N	34.84514676225609	-27.51691165616635	3.84306067749726
C	32.91015560359574	-26.55147637941261	2.69763939237100
C	32.88902614031257	-23.93875426919351	6.76721956401612
C	36.34373977034878	-26.76563897103752	8.61824735365387
C	36.81210607651636	-28.90117864930797	4.30791877994048
C	30.62927168326028	-22.73187315343030	5.04417387550132
C	33.33449553838516	-22.86626498342849	9.63724538112950
C	38.66536808782836	-28.77795873635096	8.98445957640876
C	36.36647657818335	-29.97771217508478	1.44822373322800
C	32.55742620934013	-25.62111423016553	3.66971897388012
C	33.82824492405742	-24.48279996284777	7.63788680741636
C	36.77715127055522	-27.60829532226098	7.60153144301305
C	35.78501771070260	-28.44626468748948	3.49007159226825
C	31.49310901522704	-24.64421460274741	3.52612152589915
C	34.04964300308461	-24.02050971771547	8.99938499375900
C	37.88205042131232	-28.54328708609612	7.72653635477266
C	35.53333693388370	-28.94512528721623	2.14720760552576
C	31.51420115051597	-23.88216949651322	4.66509530815999
C	35.00115315590321	-24.84604662244002	9.53750774060955
C	38.03970672846336	-29.12012489881075	6.49381974576785
C	34.39994880371719	-28.31758057751089	1.70790862130008
C	32.58000616637764	-24.41456813563899	5.49732570640160
C	35.36118047052046	-25.78939248870941	8.49243268899293
C	37.01583967170807	-28.54405044986024	5.63681815327235
C	33.98834453173938	-27.42444629002534	2.77747431288424
N	36.26905916217494	-27.63010877950795	6.32805266749101
Fe	34.69453448559155	-26.59242202396364	5.61763156058800
C	33.72017326629767	-31.50239352540961	7.11891576466304
C	35.11684982420093	-32.04263908053630	6.85058493977731
C	32.07665713317988	-27.53223976211672	6.86216730587758
C	33.43243555872775	-27.91766486793116	6.34044376371702
C	33.57209930077764	-29.35558497524617	6.05757741017095
O	33.50132628264874	-29.91517061235070	4.98272176785294
O	33.71512602687969	-30.06606060743177	7.22742810631947
H	29.90949928401099	-22.50053488875034	4.25285010912088
H	31.20791423417236	-21.81892339589166	5.23817853208810
H	30.05447157793516	-22.94651793832540	5.95500126806392
H	31.14808285114430	-24.35089124838412	1.40996903495200
H	30.01194581614111	-25.46054612801170	2.18008178691217
H	29.86722797106567	-23.72116917653175	2.45047736016187
H	33.50745138963336	-27.52746691676376	-0.09874124760467
H	34.22727223783973	-29.13014002441971	-0.28124012080597
H	32.68390606961855	-28.94472726853132	0.55828315899720
H	36.04976413140565	-30.11182249843193	0.40916616618239
H	37.42964197844046	-29.70402984270685	1.43461376285552
H	36.29119538968045	-30.95597427050336	1.94155570058807
H	33.70241570774601	-22.67753092805199	10.65052384967453
H	32.25372886576831	-23.04798492275210	9.70994758982879
H	33.46566271364591	-21.94023187310306	9.06172126110511
H	36.68871188648205	-24.71332535895756	10.88365257181472
H	35.38897821459924	-25.75989626892963	11.45784795475716
H	39.48219455115080	-29.48763949532411	8.82134904638076
H	39.10962483500898	-27.84928279015589	9.36718295841222
H	38.03345772930316	-29.18468965353434	9.78530753157069
H	38.54432438486665	-31.09925241642333	5.78884124470416
H	39.59954171563242	-29.82388269844138	5.17419329769236
H	39.75985661294130	-30.37397245283258	6.84551493196591
H	35.19758591846419	-24.00488067678360	11.51382113066290
H	39.81610808456891	-22.95570370657036	4.31563020741738
H	38.70962520467505	-21.65776806073187	4.79912267792971
H	39.30769370416104	-22.80694251164638	6.00307525088899

H	35.81894836696902	-31.69500987363348	7.61307550486272
H	35.10955423652690	-33.13811756225668	6.86055911377845
H	35.47218617166024	-31.70977198631120	5.87393525426830
H	33.02923999654764	-31.80525992575152	6.32962848912735
H	33.33986529749813	-31.85228255847132	8.08157509749246
H	32.08942128405009	-26.58275361469513	7.39961275335084
H	31.34357099179872	-27.43055962496449	6.04597725603633
H	31.69038397097027	-28.29988184783170	7.54530417369776
H	37.38528049052709	-23.22171700378024	2.67205712789221
H	37.31697013405250	-24.71062903611985	6.60077519099273
H	35.47613303588818	-24.91154879708978	2.84622401123081
H	32.31355814067938	-26.57672201421391	1.79164889426993
H	36.83759788598490	-26.85332695825817	9.58051539603144
H	37.48386803509486	-29.64317460297328	3.88897869158521
H	32.31153540950793	-23.09509782720819	7.13099770057464

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B3LYP Scan/Melmid IPC Model/Triplet/110 degrees Constrained Optimization

C	38.99114890921949	-22.76460806496520	5.00342357632660
C	37.81365924320712	-23.65092068708310	4.76050369365810
C	37.12984827219388	-24.51999862171028	5.57132299690591
N	37.16345714992349	-23.73386364145311	3.53564939255120
C	36.14300474413616	-24.62431612961378	3.65394861392317
N	36.09964807331543	-25.11458165359183	4.87398216082151
C	30.62685236479876	-24.49017145787825	2.26672825825165
C	35.50550700435048	-24.86486296361363	10.91714313625790
C	38.99505542416581	-30.16759936111695	6.06959996845711
C	33.69714702165370	-28.46234500069711	0.37390197494256
N	33.19288795848838	-25.44900218452313	4.83836252170966
N	34.60565941427918	-25.55274237867712	7.33545323668987
N	34.83513683835027	-27.51552815096918	3.82737633152517
C	32.92594736818938	-26.52550031677743	2.65804321223201
C	32.86613767826808	-23.93311953248953	6.73722657750702
C	36.28899737941097	-26.78238345441828	8.61924662127329
C	36.78924001650265	-28.91039052065434	4.30952523097397
C	30.64059052670053	-22.69704327451196	4.98477625063905
C	33.26630102133731	-22.88970030441320	9.62005754661290
C	38.60412770126783	-28.80067996396387	9.00003613431724
C	36.36563617610518	-29.97954021531440	1.44119191716922
C	32.56754372313986	-25.59574634458113	3.62781688422645
C	33.79124394378216	-24.48810106065585	7.61551315122957
C	36.73258673784854	-27.62061331397010	7.60361894825341
C	35.77134913907090	-28.45140023728298	3.48230221066848
C	31.51336949101893	-24.60884625969623	3.47120968566645
C	33.99120002167955	-24.03834531545874	8.98324079167399
C	37.83320921250905	-28.55952830681739	7.73577726482609
C	35.53156471683344	-28.94440085849108	2.13545176688789
C	31.52157208967510	-23.85291498430602	4.61371844025708
C	34.93328593440704	-24.86949228038021	9.53043570086360
C	37.99946861935360	-29.13313247630690	6.50293709584980
C	34.40924415865830	-28.30469770090719	1.68426649539936
C	32.57138054126964	-24.39793599214688	5.45980568604890
C	35.30979671086700	-25.80386072117255	8.48453029060978
C	36.98411796294751	-28.55175761364449	5.63907404848043
C	33.99236389142758	-27.41150705377102	2.75144671589726
N	36.23539891596733	-27.63567544249078	6.32589951094255
Fe	34.67678364265034	-26.58517546163824	5.60171105233272
C	33.82697193180557	-31.46595736103163	7.14349254127849
C	35.16901955446810	-32.01371162829155	6.68037432193074
C	32.22669700575337	-27.53946160601381	7.15924163307220
C	33.40287036919899	-27.90924684948070	6.29758380974099
C	33.56022320576851	-29.34664496447533	6.04630999384865
O	33.38935743919598	-29.93854414437704	5.00003197243052
O	33.82586308146706	-30.02726631083126	7.21449413518163
H	29.92760170170100	-22.46311781317613	4.18805553857327
H	31.22298058689144	-21.78690684207361	5.18130838485304
H	30.05831649090243	-22.90696108148965	5.89189993326672
H	31.20529832340525	-24.31290388707306	1.34995492079507

H	30.04091836419817	-25.40451613408672	2.10373470281822
H	29.91846307918180	-23.66250383888028	2.36998464811340
H	33.54466306543451	-27.49790195394421	-0.12844166114303
H	34.25982291942044	-29.10230244319180	-0.31286266945625
H	32.70614645095276	-28.91625907719689	0.50715623735177
H	36.06716339530213	-30.09827952068726	0.39486831200680
H	37.43175048395102	-29.71763087445814	1.45027831410410
H	36.27054930729478	-30.96260963371277	1.92131955035723
H	33.61052462255542	-22.71693422045454	10.64441042280242
H	32.18348523921190	-23.06771580927865	9.66414619168732
H	33.41516882248663	-21.95611425650159	9.06128415173766
H	36.59682408285335	-24.74188130334422	10.90700864544096
H	35.29446474010156	-25.80400196081505	11.44574206266890
H	39.42379219010025	-29.50793027938521	8.84056352739989
H	39.04271873581509	-27.87376537067834	9.39324967955535
H	37.96479617424824	-29.21398528569022	9.79159576836351
H	38.50448509917573	-31.11044082783819	5.79298918604586
H	39.56948352399728	-29.83541190967067	5.19488183301732
H	39.71209783993276	-30.39427138958474	6.86494306127991
H	35.09042043277103	-24.05109062217435	11.51968588196644
H	39.83885895338888	-23.01518639015654	4.35173669956009
H	38.75080530614375	-21.70484617079643	4.84366340145503
H	39.32646625825228	-22.87455687104233	6.03867167910600
H	35.97859983771309	-31.63436218043858	7.30942519222577
H	35.17279725068467	-33.10783778205122	6.73222065930822
H	35.36148561463633	-31.71547098011479	5.64894295007616
H	33.02656612287390	-31.79213691796843	6.47595586867884
H	33.5987926779279	-31.79013813951716	8.16153816466631
H	31.82719431426979	-26.55758310226987	6.90241156220554
H	31.40878427659713	-28.26570753462508	7.06363059006479
H	32.49403006290615	-27.50327103601816	8.22711696366259
H	37.40569247187597	-23.22283659355540	2.69878192205863
H	37.30806913194559	-24.75701391839635	6.60958311261111
H	35.47102843687395	-24.88555086628178	2.84977035152140
H	32.34271281101925	-26.54179394486998	1.74321608333869
H	36.76918726839063	-26.87644495480303	9.58774596013809
H	37.46112597713017	-29.65593123360047	3.89728403922371
H	32.28821221399269	-23.08936897445315	7.10002837615368

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B3LYP Scan/Melmid IPC Model/Triplet/120 degrees Constrained Optimization

C	38.98233120382299	-22.72497062766057	4.98062035975675
C	37.80443262035208	-23.61390451376203	4.74957672567461
C	37.14686315449732	-24.50492917916021	5.55844389226340
N	37.12384351394060	-23.67493063839229	3.54002913647722
C	36.11244201184776	-24.57471285476795	3.66476308340275
N	36.10311925575619	-25.09147065796513	4.87455412835308
C	30.60032700567806	-24.54408624272133	2.29202771211083
C	35.56067503740356	-24.82769901908033	10.90145113025273
C	39.01600053788182	-30.16886132067207	6.07362749336749
C	33.74765073063344	-28.44007546214290	0.36344546701314
N	33.19845856826527	-25.46404710572935	4.84572973100022
N	34.62532606946375	-25.55076465934542	7.33584364481032
C	34.87241081682263	-27.49595285225165	3.82182589560137
C	32.94413968192556	-26.53320487662127	2.66099756359918
C	32.86252045817190	-23.95276915939722	6.74689222681130
C	36.32606645244276	-26.76373285215433	8.61366747430649
C	36.83101945631998	-28.88617444006812	4.30312196059393
C	30.60043528839965	-22.75628786887415	5.01370992992446
C	33.28724661630407	-22.88395822427867	9.61678840375765
C	38.63335114555402	-28.79127882400121	8.99939911192530
C	36.43301208201722	-29.93032827258948	1.42581323070996
C	32.56999102095345	-25.61681079073630	3.63744426030535
C	33.80365034090624	-24.49206813801624	7.61790505013038
C	36.76609590352153	-27.60683175123848	7.60051047061977
C	35.81807654218477	-28.42084731645729	3.47389594165753
C	31.49718152713539	-24.64889723636796	3.49017938513178
C	34.01438469260775	-24.03130209339183	8.98004574167436

C	37.86388628904147	-28.54915147385325	7.73446362772881
C	35.58711809565074	-28.90729181970892	2.12344472838457
C	31.49928896645367	-23.89560440514888	4.63453410469149
C	34.97041357231315	-24.84992586249387	9.52240309589457
C	38.02772847785129	-29.12591763768049	6.50299928033665
C	34.45757740709762	-28.27913575829361	1.67458797077692
C	32.56373335206791	-24.42395904392469	5.47284195918198
C	35.34306580277317	-25.78872420894906	8.47940085268650
C	37.01669817121648	-28.53994576178688	5.63696088111292
C	34.02819672590749	-27.39831822306883	2.74677613631374
N	36.26801697697481	-27.62359099140667	6.32301640954919
Fe	34.69799954336514	-26.58434410655559	5.60131108434217
C	33.58864072998815	-31.52497381660992	7.02375744406730
C	34.98030559629004	-32.09970295624539	6.80000626956259
C	32.28966804373486	-27.55233896775073	7.19056062464585
C	33.44490109523927	-27.92633183899566	6.30223987619038
C	33.57170866334506	-29.35154432785347	6.00110375292670
O	33.54277564227118	-29.89499268791406	4.91388192618137
O	33.61826449415934	-30.09408040020297	7.16616214840967
H	29.87924903903408	-22.53246900070614	4.22146583973959
H	31.16803720500476	-21.83673195960004	5.20969519718287
H	30.02669638400527	-22.97850296401715	5.92335565609851
H	31.16862824395484	-24.35294714697051	1.37169611466814
H	30.03133002571191	-25.46931172464904	2.13038864279860
H	29.87643789753622	-23.73088687958356	2.40258093995102
H	33.57026204182867	-27.47450812878030	-0.12825611822618
H	34.32508570984928	-29.05852261182912	-0.33081668030285
H	32.76858342972188	-28.92038132235848	0.49298411267597
H	36.14074280405141	-30.04392015686973	0.37715279223846
H	37.49693437240972	-29.66022332860434	1.44241348989070
H	36.34262292693625	-30.91726459168509	1.89889038680946
H	33.64196114541353	-22.70065867938347	10.63571781849163
H	32.20650168289428	-23.07046765475229	9.67492209199578
H	33.42187857190913	-21.95347516904848	9.04931782568699
H	36.64966924788463	-24.68740376811214	10.87574383907058
H	35.37193010369715	-25.76664502284457	11.43872352637198
H	39.45336915333979	-29.49815138397454	8.84016250805055
H	39.07151952444168	-27.86449972792235	9.39350579603599
H	37.99361243099438	-29.20516262273570	9.79036870265110
H	38.51886919945628	-31.11112112314861	5.80669714083752
H	39.58884684163591	-29.84726418007033	5.19395849806149
H	39.73498368226969	-30.39322181061787	6.86786655119503
H	35.14071345000446	-24.01684044259756	11.50452012532987
H	39.81408032799433	-22.95589649262294	4.30163330385115
H	38.73114699637064	-21.66375292247740	4.84968305076100
H	39.34569336281847	-22.85438781680639	6.00408680565086
H	35.65929888757055	-31.79149318369353	7.59967070629101
H	34.94292513870395	-33.19449305602078	6.78169172377643
H	35.38481886690448	-31.75277460883046	5.84773591357843
H	32.92361311826324	-31.79114139620557	6.19935059412813
H	33.15924867987523	-31.88734169388720	7.96103607888005
H	31.85289990647015	-26.59504585344006	6.90148345159535
H	31.49443084879984	-28.30686202191523	7.16617229445774
H	32.59800069097427	-27.45232478319270	8.24246472562439
H	37.34147486793355	-23.14430609793442	2.70861311084042
H	37.35284327731653	-24.76287854156300	6.58656171398426
H	35.42227588913434	-24.82328161410982	2.87206837066869
H	32.35892608243983	-26.55575882054131	1.74757711940689
H	36.81163998011281	-26.85122727579350	9.58013194128632
H	37.50570390218049	-29.62783577669312	3.88851664279046
H	32.27629166660117	-23.11618147012468	7.11297003091083

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B3LYP Scan/Melmid IPC Model/Triplet/130 degrees Constrained Optimization

C	38.94846524614283	-22.68930617404061	5.01529382771518
C	37.78588369783255	-23.59217468465214	4.76164537029206
C	37.13209632366834	-24.50057810186757	5.55411509330767
N	37.11882439418466	-23.64948095816231	3.54436903312559

C	36.11890335714416	-24.56454348414866	3.64888842026339
N	36.10400232963048	-25.09417559052800	4.85302922753194
C	30.61772848676939	-24.49534063232459	2.27458840939063
C	35.51518988482964	-24.97760616035509	10.90613110322704
C	39.08116626910391	-30.11673406648712	5.93607528600430
C	33.73742563261622	-28.39298646441855	0.29700016090685
N	33.20837884034824	-25.46643482387416	4.81636385302721
N	34.62537414969606	-25.60117604328714	7.31051033817513
N	34.87650248981215	-27.48477153019316	3.76056529935905
C	32.93908173425799	-26.51482021493689	2.62229389235145
C	32.87713324863172	-23.98163759507056	6.73985208610326
C	36.31967004183455	-26.84079965856697	8.56865893795049
C	36.86337834334314	-28.84412909049368	4.20377197154026
C	30.64080842133472	-22.73212619602271	5.01180048999573
C	33.26713162386020	-22.99021267981493	9.64288019158385
C	38.66237209391439	-28.83626609948036	8.90185815163024
C	36.44955853017913	-29.86491110531665	1.31940454081748
C	32.57665964263029	-25.60258177515648	3.60760409878393
C	33.8039988705053	-24.54744198595472	7.60925000117143
C	36.77625374107649	-27.64803594458228	7.53344466781532
C	35.83337098128071	-28.38874344136752	3.39142006454917
C	31.51415645036945	-24.62227594059654	3.47094228930966
C	33.99936349828005	-24.12280791640690	8.98593123645375
C	37.89095958567351	-28.57267404269023	7.64240222934627
C	35.59657980836383	-28.86169468100474	2.03672654580990
C	31.52591393568933	-23.87883127662317	4.62217827198076
C	34.94538201763939	-24.95885306058360	9.51859383861544
C	38.06847328787993	-29.11010730890628	6.39462561843516
C	34.45441230267078	-28.24391483678021	1.60582136884495
C	32.58375868898364	-24.42689820182878	5.45520762454419
C	35.33028754998877	-25.86974832476113	8.45478736219161
C	37.04660658206318	-28.52234978630724	5.54362511192384
C	34.02408225495805	-27.38042785786626	2.69265480296164
N	36.28030788761521	-27.63941295030537	6.25436097389848
Fe	34.70367221298213	-26.60329927383397	5.55719968594112
C	33.50285903774265	-31.48110822842842	7.24547598672748
C	34.91624770136318	-32.02045130697101	7.41326092169114
C	32.22934059311721	-27.55926045439221	7.04559431187821
C	33.45175792274987	-27.94532486148300	6.25798823478689
C	33.67281212386473	-29.37784937563038	6.09174081801577
O	33.90233498446913	-29.99373929991982	5.06759116828108
C	33.47253163319996	-30.04534748265862	7.28927209831554
H	29.92036828285868	-22.49445779148633	4.22296850590053
H	31.21942230097149	-21.82059695359628	5.21296775072202
H	30.06673889269012	-22.95440025881081	5.92118365702695
H	31.18708854726482	-24.29550592311290	1.35674288267277
H	30.04238247113742	-25.41435284566200	2.10055250812846
H	29.89931237410340	-23.67893239928352	2.39646477747759
H	33.56703311373862	-27.42332206499807	-0.18945497776429
H	34.30655760265543	-29.01311814083823	-0.40250738643364
H	32.75412680123380	-28.86442504398148	0.42714640464485
H	36.14393504263457	-29.97670117676079	0.27435308650584
H	37.50892471599414	-29.57680342462372	1.32241534806021
H	36.38270284737904	-30.85578135924294	1.78790911621936
H	33.60574906342845	-22.83703137560573	10.67220219983414
H	32.18484333555194	-23.17319453663325	9.67820549020462
H	33.41489011295351	-22.04476348914817	9.10407694655463
H	36.60703198294854	-24.85968178240651	10.89927972805182
H	35.29893209159214	-25.92346723397977	11.42052328991354
H	39.48761215844437	-29.53346740016612	8.72788827284304
H	39.09335084466557	-27.91502865629328	9.31631036551756
H	38.02517711253968	-29.27183235564440	9.68319315595319
H	38.60507262327157	-31.05572700691072	5.62368761605839
H	39.65786715924482	-29.74773915194298	5.07777915166696
H	39.79431187778021	-30.36069520500060	6.72962166136719
H	35.10304966071052	-24.17085335383575	11.52006740318366
H	39.78868313822969	-22.89705066224204	4.33925247065951
H	38.68220206730911	-21.63006985749785	4.89880088645111

H	39.30597314565129	-22.82910306725305	6.03943441475250
H	35.36983051611783	-31.63728456385384	8.33138851595267
H	34.90404194598645	-33.11468538833325	7.46696115469199
H	35.53905425348925	-31.72299203783329	6.56776091663740
H	33.06861078808949	-31.82256268493438	6.30361117796437
H	32.86090746301125	-31.79800204863053	8.07134548298535
H	31.80335257646724	-26.61765500137505	6.69849870054279
H	31.45070510540096	-28.32846591518049	6.99084708535285
H	32.46128126254619	-27.42637589916778	8.11328437640984
H	37.33776532763689	-23.10719678754755	2.72085885001348
H	37.33135668789909	-24.76703774287765	6.58137820214328
H	35.43999017938149	-24.81362279585054	2.84672613284388
H	32.34875225172448	-26.52672373311941	1.71188374258573
H	36.80067246783378	-26.95109533419084	9.53504077737266
H	37.54928324175886	-29.56576645042687	3.77276828035014
H	32.29467409983641	-23.14737622364007	7.11705056140942

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B3LYP Scan/Melmid IPC Model/Triplet/140 degrees Constrained Optimization

C	38.94316247548901	-22.68414510411019	5.02028163183411
C	37.78100403628324	-23.58684156287838	4.76401789071018
C	37.13225456356238	-24.50336854721343	5.55125690597802
N	37.10881315749221	-23.63473866704526	3.54911876086302
C	36.11068958019967	-24.55220487558017	3.65011687179082
N	36.10197101667717	-25.09236935969668	4.84956965026274
C	30.59817774625719	-24.52367414368510	2.28379296000946
C	35.51586667265294	-24.99934515102622	10.90100618577607
C	39.10607129734043	-30.09699429708790	5.90708457371028
C	33.75408755273434	-28.38201715028042	0.27984722555410
N	33.20864052420070	-25.47850656090363	4.81094996023203
N	34.63070536066891	-25.61323499464285	7.30281297546161
N	34.88675426792781	-27.47983646679492	3.74733019595648
C	32.93484878134407	-26.52814502811309	2.61845360206960
C	32.88550586061853	-23.98981666721895	6.73296918549884
C	36.31717446708385	-26.86252832926888	8.56143378828623
C	36.89182080414881	-28.81589748830740	4.17839878330192
C	30.63418585868338	-22.75151976558123	5.01537820765293
C	33.28164557323847	-22.99791949707413	9.63532758672105
C	38.66096639993787	-28.85857621913862	8.88733303791974
C	36.49248397294816	-29.81663580996474	1.28609810575953
C	32.57040318749176	-25.61922179519200	3.60627990078004
C	33.81346175881708	-24.55605364068701	7.60117090531100
C	36.77764675896420	-27.66227242491835	7.52215612264379
C	35.85671927764435	-28.36610377848975	3.36986329615838
C	31.50310988329087	-24.64361929968426	3.47446005478627
C	34.00929247956709	-24.13339978554759	8.97827327847991
C	37.89583751950941	-28.58320477160855	7.62657333827979
C	35.62471771060154	-28.83257532565405	2.01224205608829
C	31.52049550071807	-23.89641004279682	4.62327061573969
C	34.94935046299447	-24.97560777331043	9.51216246517054
C	38.08455942896774	-29.10263574333366	6.37278808345747
C	34.47125663751207	-28.23074484075534	1.58837522725512
C	32.58522953282178	-24.43902768577228	5.45109745927431
C	35.33208072293455	-25.88676293651119	8.44799267309257
C	37.06415918231984	-28.51041960437268	5.52319173204520
C	34.03047518910975	-27.38083763871204	2.68177906762391
N	36.28757834638471	-27.64231339315351	6.24054981554169
Fe	34.70760473877510	-26.61250393911007	5.54828574678035
C	33.42174086101571	-31.49366625934644	7.22263857809436
C	34.82309682822989	-31.98567965264780	7.55740624984874
C	32.25424761414233	-27.55215876398851	7.07004137153162
C	33.45208982645772	-27.95098816905601	6.25295138194232
C	33.68047179346360	-29.38140777748767	6.10480845650427
O	34.04535997133488	-29.99064746786222	5.11497071143788
O	33.33804759716592	-30.06106191292186	7.26558835711764
H	29.91080815056133	-22.51568144594899	4.22869986324142
H	31.21149948388911	-21.83870002166207	5.21432923921529
H	30.06342827997127	-22.97464501292930	5.92665386639433

H	31.16020550086796	-24.32184377311486	1.36185541041085
H	30.02728518312351	-25.44641559315866	2.11492555672505
H	29.87559062246584	-23.71149020568029	2.40916951130355
H	33.57037850570842	-27.41210809819345	-0.20122424930222
H	34.33022040573950	-28.99105444190569	-0.42370056705731
H	32.77719451220428	-28.86696609031763	0.40871300517118
H	36.18546014920337	-29.92756155767916	0.24137235533726
H	37.54665810469540	-29.51003427692268	1.28774135006199
H	36.44455428976034	-30.81123449447037	1.74899057418393
H	33.62262256283987	-22.84473046904539	10.66387329691499
H	32.19886772215237	-23.17765887369960	9.67290548356639
H	33.43123381112907	-22.05351470904946	9.09525556209732
H	36.60848633879724	-24.88887099281136	10.89684000842462
H	35.29192369462827	-25.94411764970578	11.41412334005454
H	39.48803935692531	-29.55294896849444	8.71074306977999
H	39.08867870729049	-27.94098107819091	9.31317351819516
H	38.02024951836101	-29.30270970169178	9.66089291150128
H	38.63682675700665	-31.03230265242073	5.57419768074743
H	39.68920853576140	-29.71079639290055	5.06074542557683
H	39.81273325419044	-30.35125413059631	6.70317442730463
H	35.10775311160270	-24.19033884798914	11.51468495894208
H	39.78110484873515	-22.88530098571527	4.33942750300390
H	38.67480197026889	-21.62446404542698	4.91301518701664
H	39.30487230835389	-22.83128075679985	6.04191799681719
H	35.14879185774925	-31.59351677064122	8.52488337940848
H	34.84401060459384	-33.07998764223124	7.60617549552772
H	35.53249954508243	-31.66016903059729	6.79469671824072
H	33.11518469815272	-31.84456204854815	6.23516769768081
H	32.69731863055012	-31.83732086475774	7.96546875169040
H	31.83942607693400	-26.59806036073584	6.74572942319651
H	31.46238937683738	-28.30732065506859	7.02236537027723
H	32.51248863072264	-27.44043068396829	8.13381037975335
H	37.32330855730817	-23.08485838592561	2.72948544864153
H	37.33623184714428	-24.77841372821775	6.57532452786219
H	35.42865342855895	-24.79520604033822	2.84875038906241
H	32.34101309113770	-26.54381444600959	1.71039073135883
H	36.79484227718515	-26.97876165061203	9.52877144829614
H	37.58734181327942	-29.52467138727229	3.74155242618387
H	32.30476808380659	-23.15459702302307	7.11070019685754

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B3LYP Scan/Melmid IPC Model/Triplet/150 degrees Constrained Optimization

C	38.91699550937081	-22.64303182494227	5.01135477436985
C	37.76695132137883	-23.56068731593535	4.75359549898709
C	37.12735492080546	-24.48406102760223	5.54032960427122
N	37.09848716137513	-23.61832422957892	3.53709478282021
C	36.11153513951876	-24.54799193469037	3.63666014930183
N	36.10614469881850	-25.08652990859066	4.83683287247988
C	30.58638589540892	-24.54912699594892	2.30355100213171
C	35.52303318638011	-25.05604552188927	10.90287977161185
C	39.17235266763110	-30.04463385267087	5.84057264538019
C	33.76116409983047	-28.37834986826281	0.26352887423786
N	33.22338261295831	-25.49202891719688	4.80696821944717
N	34.65008873187983	-25.63640557147582	7.29660904476986
N	34.90281939384292	-27.47996727704560	3.72966952593081
C	32.93298582098724	-26.54547273655568	2.61824549612045
C	32.90734819757711	-24.00786021145480	6.73437549878732
C	36.33703596478518	-26.89327395185554	8.54508918152770
C	36.94222839739304	-28.77059801830934	4.13247550877375
C	30.64610659171253	-22.76935690431329	5.02971366396500
C	33.29575909386011	-23.04011639190034	9.64689002780717
C	38.70156656124141	-28.86973635582459	8.84325347091742
C	36.53884566546363	-29.76030884947964	1.23572013373319
C	32.57414581400530	-25.63671943157272	3.60868162260716
C	33.83269131056412	-24.58104193447750	7.60088540377107
C	36.80685459769955	-27.67282884275615	7.49457695105795
C	35.88971554041188	-28.34024336563697	3.33643417478311
C	31.50352642402872	-24.66414412638744	3.48541243639381

C	34.02492963900738	-24.17025237522419	8.98236402878327
C	37.93619003449263	-28.58143022738513	7.58547683312622
C	35.65612014660171	-28.80093861779190	1.97689664355697
C	31.53105711505729	-23.91348513027308	4.63219012258225
C	34.96185777853373	-25.01842906944409	9.51218943157488
C	38.13659331340900	-29.07292741002495	6.32211784689183
C	34.48599834344704	-28.22118507889054	1.56729882069358
C	32.60335490432739	-24.45303663040888	5.45163177157649
C	35.34836109769239	-25.91986904404407	8.44091652843151
C	37.10986566812767	-28.48045536513333	5.48089870773796
C	34.03771660060185	-27.38715733721817	2.67023542808200
N	36.31970239667650	-27.63692627678224	6.21200598602629
Fe	34.72820200194201	-26.62391916940332	5.53690823527910
C	33.29145657262429	-31.50005105528149	7.21639195992414
C	34.58902296322552	-31.95880346318977	7.86772501806878
C	32.23991758048339	-27.55343225854481	7.00132833257816
C	33.47687565526947	-27.96026309647447	6.25000449886579
C	33.73691893381350	-29.38766190211652	6.16081565290912
O	34.30666342595097	-29.99818313363759	5.27162699438798
O	33.17088949626861	-30.07086650159312	7.23138055683370
H	29.91770882363045	-22.53443460718180	4.24743538504743
H	31.22385793296440	-21.85599909909252	5.22473848194093
H	30.08115981349792	-22.99274412849637	5.94453841555199
H	31.13793201350479	-24.34289638310299	1.37624791781145
H	30.01990040809500	-25.47544477866227	2.13959453950467
H	29.85961826798638	-23.74190928400713	2.43662449571036
H	33.54198983322613	-27.40868992746580	-0.20273303198813
H	34.34971771020513	-28.95941989814065	-0.45335685253352
H	32.80141709127843	-28.89607401027055	0.39452694976392
H	36.22391611805507	-29.87180467468101	0.19339057516683
H	37.58557829553148	-29.42919673471619	1.22919760624006
H	36.51903885757117	-30.75863178775741	1.69262477739657
H	33.63366569568829	-22.89591386682149	10.67775297555666
H	32.21281314092775	-23.21981260542124	9.67966751885733
H	33.44728991334203	-22.09113222077241	9.11546082746293
H	36.61616354267807	-24.95094172671731	10.90373837928612
H	35.29249000497037	-26.00392737723336	11.40731377168458
H	39.53076656842484	-29.55951941110411	8.65867005803655
H	39.12661946387689	-27.95591766799456	9.27990733254156
H	38.06191025741924	-29.32479417459228	9.61117474602699
H	38.71502869802897	-30.97757861850999	5.48561645274702
H	39.75439891353135	-29.63293172325866	5.00553626096097
H	39.87850515266575	-30.30714663150897	6.63441625227310
H	35.11649365630078	-24.25008204003365	11.52161536441402
H	39.75834590410697	-22.83345267042768	4.33162130441747
H	38.63500764970743	-21.58694812457394	4.90344618185178
H	39.27923260636458	-22.78520781231986	6.03349769319430
H	34.66679152804767	-31.57094511704550	8.88737267235040
H	34.63063280765119	-33.05266621424376	7.91262914275491
H	35.44809864161632	-31.60437043772618	7.29509878633388
H	33.22963248531735	-31.85661429133350	6.18647662034842
H	32.42357365469193	-31.86195944233081	7.77388170254124
H	31.85778068877349	-26.58757364761193	6.67603738710477
H	31.44262110868430	-28.29637211973711	6.89644091889946
H	32.44005453088634	-27.46936520872982	8.08019459690834
H	37.30818507427065	-23.06666353211568	2.71740847383815
H	37.33192209027693	-24.75518181872680	6.56533142893415
H	35.43410676938388	-24.79943394295213	2.83401567519627
H	32.33161370912292	-26.56389471019333	1.71519941885370
H	36.81369506601550	-27.01934245349796	9.51168776732065
H	37.65142364658036	-29.45883623665203	3.68495135637942
H	32.32691986361975	-23.17440642602376	7.11646963941762

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B3LYP Scan/Melmid IPC Model/Triplet/160 degrees Constrained Optimization

C	38.91383179716058	-22.63393453833754	5.00012711641944
C	37.76304617019198	-23.55222201069703	4.74792566961615
C	37.13236184639651	-24.48092103711894	5.53553163235057

N	37.08400844961165	-23.60507508328415	3.53704953305022
C	36.09957270545796	-24.53701485851384	3.64080310060717
N	36.10599249991580	-25.08175029601967	4.83812536654198
C	30.56683821135984	-24.59317620401567	2.32357637495930
C	35.53795987906782	-25.04411448352241	10.90299583627107
C	39.21087012494129	-30.00870827908529	5.83606416292165
C	33.76867046891298	-28.39961637056145	0.27749568859083
N	33.22567649063438	-25.50591776150658	4.81471126897589
N	34.66208103556674	-25.63560270836006	7.29956933736363
N	34.91456691035239	-27.48341983704958	3.73730912661794
C	32.92786380967734	-26.57425747380484	2.63461651341822
C	32.91896812239241	-24.00837844646044	6.73310215318351
C	36.34942339646667	-26.88966925475875	8.54996159855964
C	36.97581969102367	-28.74202246180256	4.13042503693862
C	30.64181542960747	-22.78956078136132	5.03396242772838
C	33.31607801711770	-23.02661197320107	9.64022671532692
C	38.72363054631826	-28.85590355749544	8.84501766082011
C	36.57441210472926	-29.73550303525863	1.23410864915269
C	32.56875069600676	-25.66241760464360	3.62229715390064
C	33.84713682152727	-24.57696684767031	7.59990213938119
C	36.82375467344003	-27.66467696751327	7.49805617882494
C	35.91369298148925	-28.32716091797137	3.33879910761323
C	31.49335395246303	-24.69487727252262	3.49932937747463
C	34.04166313500188	-24.16128489973424	8.97948401172491
C	37.95980778406632	-28.56560786965825	7.58672084183394
C	35.68010036447252	-28.79087851512226	1.98040390142076
C	31.52735167015118	-23.93419765847829	4.63929333038707
C	34.97612618875283	-25.01046893722844	9.51243210616268
C	38.16793102211680	-29.04652149786875	6.32080343828835
C	34.49798059989261	-28.23054082596357	1.57734218705338
C	32.60730244728963	-24.46374145255036	5.45549208565424
C	35.36048964696973	-25.91641621547325	8.44436097342191
C	37.13831401009889	-28.45731198746149	5.48048131135170
C	34.04275559635617	-27.40294817994369	2.68217586950107
N	36.33923680088429	-27.62564931578618	6.21486069809548
Fe	34.73896261261059	-26.62804870052616	5.54337229434207
C	33.19179782536693	-31.52931752533552	7.10083589067095
C	34.42397951907432	-31.98158490061057	7.87292086248000
C	32.27327247754366	-27.54825121706754	7.03929425419416
C	33.48900119702640	-27.96363906323197	6.25953713253653
C	33.74218673213868	-29.39023472908423	6.16166712472973
O	34.430444416174617	-29.98070737571670	5.34429873292221
O	33.04285742006080	-30.10359938847041	7.13005868737845
H	29.91000436581711	-22.56014792186838	4.25323242497810
H	31.21865714921371	-21.87415443294422	5.22186112745355
H	30.08073421794620	-23.00899383303637	5.95214266968069
H	31.11075387934060	-24.39489342256863	1.39006206518887
H	30.00108561578467	-25.5222367192010	2.17298965995210
H	29.83933188240056	-23.78623799549529	2.45437564387278
H	33.53097511134408	-27.43363431002626	-0.18727342041084
H	34.36287614872068	-28.97075042029288	-0.44273310492636
H	32.81834676722352	-28.93322126876877	0.41351711587283
H	36.25229926336767	-29.85649064985775	0.19504970054222
H	37.61447143694893	-29.38423559785799	1.21733481804547
H	36.57818841485907	-30.73251002195042	1.69429504399411
H	33.65746745599388	-22.87739891973754	10.66923260122730
H	32.23297791228637	-23.20462589879691	9.67737690516643
H	33.46729473520974	-22.08075290687631	9.10320298494233
H	36.63107094864738	-24.93872886615623	10.90303779733830
H	35.30794869744742	-25.99065753173421	11.41017672230268
H	39.55586549012918	-29.54179082617807	8.65948476486043
H	39.14433548255647	-27.94218921950554	9.28617725763931
H	38.08413383749991	-29.31630414296114	9.60985878904759
H	38.75932572614327	-30.94246297036142	5.47589071906134
H	39.79148520852696	-29.58908217563521	5.00397399483587
H	39.91751296402200	-30.27080090953960	6.62963309020076
H	35.13147105250891	-24.23660074944928	11.51974733196163
H	39.74976613404959	-22.82009496467658	4.31256937654852

H	38.62938312958362	-21.57782128520339	4.89923982306640
H	39.28481594642813	-22.78009784491990	6.01857263043213
H	34.38904688524121	-31.61707319846915	8.90358101768740
H	34.48142152208825	-33.07537653513164	7.89759595484848
H	35.33038412270337	-31.59974503976249	7.39970576678421
H	33.24188481350829	-31.86626360016528	6.06358074428082
H	32.27790612448776	-31.91636069453207	7.55891655632969
H	31.90874165623409	-26.56546416795630	6.74798076826112
H	31.45877579989657	-28.27042301604659	6.92698538761115
H	32.49346241260856	-27.50030735753062	8.11639869258033
H	37.28546732955153	-23.04895481985082	2.71830855324146
H	37.34676738595007	-24.75698017306853	6.55720222025909
H	35.41554466956439	-24.78565538678655	2.84288497420892
H	32.32111131882233	-26.60225594159781	1.73541893999540
H	36.82543175454433	-27.01545614632075	9.51692591419447
H	37.69442879673770	-29.41814500429419	3.67941616800806
H	32.34012537561205	-23.17254193532057	7.11240884807666

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B3LYP Scan/Melmid IPC Model/Triplet/170 degrees Constrained Optimization

C	38.92390767299613	-22.63284271054820	4.97280347374863
C	37.76606887111719	-23.54595377220834	4.73458834619389
C	37.14397577423426	-24.47521268449416	5.52826157977492
N	37.06973483490288	-23.59306353041215	3.53333253540245
C	36.08451210088415	-24.52292488318374	3.64812389347702
N	36.10653363902485	-25.07146848403593	4.84342656487092
C	30.54109801066210	-24.65052275696009	2.35396065180606
C	35.56800376032996	-24.99881944635970	10.90364902066854
C	39.25624058852831	-29.96178083240336	5.84982871397366
C	33.77128829524923	-28.43884181543163	0.31259923448011
N	33.22640865518352	-25.51941910540624	4.83213495796340
N	34.67740363950016	-25.62258326880668	7.30956066559737
N	34.92941151257103	-27.48505163123020	3.75754560353613
C	32.92242307133549	-26.60911584324363	2.66409095923363
C	32.92729955646965	-24.00414317573775	6.73730376977952
C	36.37159022917293	-26.86425977907931	8.56305199221980
C	37.01153163744358	-28.71161675736854	4.14427972783379
C	30.62823980250383	-22.81657368072384	5.04388150323009
C	33.34161513865705	-22.99238301032942	9.63197811665417
C	38.75614918719437	-28.81820350096019	8.86040186696257
C	36.60438792210160	-29.72592586039326	1.25522697738646
C	32.56143454011426	-25.69242740951186	3.64668249237528
C	33.86292827078080	-24.56154376161079	7.60362766676337
C	36.84889375810458	-27.63951947391593	7.51261932886189
C	35.93902707652058	-28.31528156341189	3.35669105463816
C	31.47815417001115	-24.73345835459382	3.52281147415059
C	34.06357661029050	-24.13351470747798	8.97835495908348
C	37.99274685579272	-28.53110326177463	7.60114168020224
C	35.70217287840215	-28.78979110910725	2.00275677366395
C	31.51703555653245	-23.96028443159547	4.65404725591367
C	34.99984623168514	-24.97842445633012	9.51535508978260
C	38.20648450416400	-29.00735455041849	6.33477113222038
C	34.50809085153993	-28.25026414846150	1.60557249367716
C	32.60694760367382	-24.47470779362553	5.46715485702478
C	35.38051709430079	-25.89330786947568	8.45385583127749
C	37.17172334868810	-28.42638014795518	5.49443080386664
C	34.04862230430510	-27.42293312391796	2.70858364943208
C	36.36422189955736	-27.60434537462980	6.22984307638228
Fe	34.75281785785592	-26.62558729321256	5.55990356232369
C	33.07026243092664	-31.56194020021339	6.91289162376686
C	34.21740543964355	-32.06582802294206	7.77871317698223
C	32.32556813206655	-27.54746479353357	7.10215571107252
C	33.50908902347146	-27.96610818903577	6.27677520353999
C	33.74563251568770	-29.39187583071921	6.14523699716983
O	34.53057893682617	-29.95928711433523	5.40043083546447
O	32.92822990346572	-30.13763840910976	6.98941625922284
H	29.89148861772978	-22.59664389123969	4.26508130802820
H	31.20191335078215	-21.89716846825946	5.22153767231541

H	30.07275412941259	-23.03102306028498	5.96662915685614
H	31.07621691425982	-24.46320997679690	1.41317413447191
H	29.97712964045629	-25.58331582910317	2.22079945729823
H	29.81204124667798	-23.84425203380540	2.48015196882931
H	33.51129546875755	-27.47955922229864	-0.15395200695317
H	34.37023809778433	-29.00157667310848	-0.41030031720774
H	32.83254236844739	-28.98997441068824	0.45884277138341
H	36.27397947644903	-29.86084047341053	0.22052035169191
H	37.63842864634189	-29.35818509302371	1.22538442646259
H	36.62876347909779	-30.71880262133084	1.72361081635705
H	33.69000286543900	-22.83208455315448	10.65694699002192
H	32.25889194380701	-23.17050886833601	9.67840585390583
H	33.48871653740456	-22.05231686886460	9.08381879771517
H	36.66044247270938	-24.88679936758184	10.89796308615756
H	35.34609640602567	-25.94304436412342	11.41864239188589
H	39.59272673396682	-29.49898372909874	8.67562428690748
H	39.17062434331177	-27.90262470652955	9.30361630398741
H	38.11786543752081	-29.28324919019063	9.62346231010003
H	38.81070290180987	-30.89881978200027	5.49070711784821
H	39.83315884812367	-29.53851367138861	5.01704638419878
H	39.96531219264772	-30.21843099136996	6.64302146497381
H	35.15935938750334	-24.18944212240250	11.51648204708802
H	39.75011946476547	-22.82220915929652	4.27446332983847
H	38.64289927725637	-21.57543577193994	4.87636723975686
H	39.30728622288119	-22.78161592993871	5.98626318577649
H	34.08850884744981	-31.74683231749894	8.81695180104695
H	34.25921526313795	-33.16043707344357	7.75958197618127
H	35.16893380925388	-31.67854382835267	7.41100174099045
H	33.21796656646205	-31.85502752721442	5.87141320816744
H	32.11273977275584	-31.95664547287336	7.26216977636632
H	31.97387811293422	-26.54977700036860	6.84916500688587
H	31.49423748174841	-28.25000208495305	6.99462094923545
H	32.58045178524200	-27.53327507809493	8.17256916243405
H	37.26130318500436	-23.03521085774478	2.71342105785936
H	37.37218858074674	-24.75506206716250	6.54589183410002
H	35.38925846611210	-24.76790817139751	2.85883291090632
H	32.30925015991399	-26.65130184681749	1.76983842335675
H	36.84948686317676	-26.98422052012259	9.52981939205374
H	37.73811622834966	-29.37802295097855	3.69157111242786
H	32.34845369687308	-23.16636054617915	7.11225167464134

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B3LYP Scan/Melmid IPC Model/Triplet/180 degrees Constrained Optimization

C	38.90907660030999	-22.60824051757459	4.94012693690132
C	37.75386083784444	-23.52828172653844	4.71621627363715
C	37.15078818423673	-24.46534323328184	5.51548703495988
N	37.03916175610046	-23.57517739038040	3.52577082441790
C	36.06196983466573	-24.51211384533611	3.65218778757684
N	36.10645492762873	-25.06557196189241	4.84461568712959
C	30.53527092082916	-24.69205278926034	2.37805860647933
C	35.60460214679257	-24.96575494080252	10.90618799180129
C	39.31939605420619	-29.90381891810888	5.85082537629268
C	33.77785388770623	-28.47088819682865	0.34282986428213
N	33.23224920495243	-25.53795305974050	4.85198362221341
N	34.69803416339012	-25.61751571270840	7.32104834891263
N	34.94241448971868	-27.50003062392120	3.78065680082234
C	32.92398918949589	-26.64235858923000	2.69219652630979
C	32.93760900115326	-24.01010664168874	6.74747484512723
C	36.40892330356481	-26.83850561124914	8.57203426266908
C	37.04474789369552	-28.69522403630697	4.15724870941186
C	30.62913303246223	-22.83913147474611	5.05469647550531
C	33.36156590132065	-22.97861193718977	9.63345240300383
C	38.81927673119620	-28.76108180528196	8.86201677840171
C	36.62858308801646	-29.72814003383520	1.27453877324242
C	32.56291855761211	-25.72101925554123	3.67049712093802
C	33.87988004408458	-24.55822374740918	7.61250966815395
C	36.88943235058407	-27.61139154160638	7.52132125706386
C	35.95937691585782	-28.32012072674456	3.37648109801707

C	31.47663653939982	-24.76544659290121	3.54409549648760
C	34.08518688841282	-24.12079600268904	8.98347796593535
C	38.04618311172192	-28.48699393342809	7.60587171164336
C	35.71955993125975	-28.80134219504868	2.02552342201057
C	31.51825125465650	-23.98422017686345	4.66965522626640
C	35.02833995167538	-24.95775352012858	9.52112454023996
C	38.25978302298986	-28.96261127552745	6.33965306864781
C	34.51781551036053	-28.27473487924352	1.63294081386082
C	32.61269047258109	-24.49044039929358	5.48204953282909
C	35.40888595024428	-25.87674587806660	8.46332056358745
C	37.21145148881794	-28.39925302277420	5.50401170519731
C	34.05594429578057	-27.44844887301265	2.73542496021530
N	36.39713460577848	-27.58611267789986	6.24164521830386
Fe	34.77090616887988	-26.63106191076170	5.57803953634565
C	32.94113591494077	-31.58374754670993	6.73228341425022
C	33.94060141701846	-32.15677118945596	7.72853312256882
C	32.36744789271663	-27.55579548418989	7.14421790453634
C	33.53484849247810	-27.97794036093783	6.29799822724080
C	33.76108826220164	-29.40405529662551	6.15220800495236
O	34.64140965206995	-29.96629209116560	5.51738793096209
O	32.82120329971047	-30.16034014981217	6.84738987208514
H	29.89079311467793	-22.62393733640969	4.27603113411550
H	31.20243777959005	-21.91832968333696	5.22634228495437
H	30.07538420801493	-23.04878938200054	5.97963069460090
H	31.06699268864433	-24.51254318921955	1.43380150137755
H	29.97054452486004	-25.62573110075077	2.25444965487849
H	29.80683511350935	-23.88455167474705	2.50022754263263
H	33.52218344848007	-27.51409950745771	-0.13141119867294
H	34.37272436299583	-29.04265224146139	-0.37631588610023
H	32.83633203220803	-29.01559129852879	0.49493770596020
H	36.28592873142688	-29.88008480914695	0.24619311558220
H	37.65489036957219	-29.34099601572812	1.22580981817860
H	36.67909142462732	-30.71534297273440	1.75264634869967
H	33.71286997362453	-22.81172994787158	10.65638860894259
H	32.27955884540295	-23.15992029869450	9.68436618596524
H	33.50385154367713	-22.04098163795160	9.07980527435766
H	36.69530046733958	-24.83780987130359	10.89386221448259
H	35.39957803938587	-25.91162468642842	11.42514364696283
H	39.65986230297152	-29.43661019490426	8.67598701774947
H	39.22938752619933	-27.84012100618155	9.29823864325157
H	38.18880693249263	-29.22686510349690	9.63114875963000
H	38.88343529318289	-30.84595500122478	5.49327529928940
H	39.88806827861544	-29.47339002878115	5.01594846435275
H	40.03446792063750	-30.15212646704224	6.64131968562452
H	35.18770333742710	-24.16063062338349	11.51906446552006
H	39.72547964673520	-22.78892674187393	4.22803419114481
H	38.61948508744297	-21.55233779929417	4.85275274444315
H	39.30951076412262	-22.75873350943842	5.94674964178021
H	33.68029158464068	-31.86536094408319	8.75010724771930
H	33.94758549173200	-33.25113909441223	7.67643761175300
H	34.94647943486633	-31.79577253357970	7.50828451584153
H	33.22837618571825	-31.84127869718082	5.71055316713187
H	31.93445605020258	-31.96344037968325	6.92537157947612
H	32.02714047975483	-26.54901135212902	6.91350481086443
H	31.52561114934880	-28.24449184858451	7.03442089830715
H	32.63767444651768	-27.56353558730278	8.21106851480315
H	37.21403718905693	-23.01250705882914	2.70541200705239
H	37.39707714450859	-24.74780436237518	6.52819136783498
H	35.35578385412326	-24.75818191320607	2.87295536192328
H	32.30749787954122	-26.69286808148420	1.80061874438727
H	36.89301702675253	-26.94990997426479	9.53674887821835
H	37.77749348985886	-29.35324946401366	3.70211726293010
H	32.35771867939260	-23.17181089874008	7.11972886061645

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B3LYP Scan/Melmid IPC Model/Triplet/190 degrees Constrained Optimization

C	38.90722719197315	-22.59237664548637	4.90846397927690
C	37.75191493348535	-23.51621638149574	4.70165867006799

C	37.16948998524036	-24.46209154582058	5.50599529557715
N	37.01293654836822	-23.55721092798482	3.52595692247135
C	36.04262285337450	-24.49939022877702	3.66531671794440
N	36.11419652471303	-25.06183989361828	4.85218998690898
C	30.51431298055055	-24.76122639805503	2.41717299703905
C	35.66043766503789	-24.91497951203974	10.90362125677497
C	39.38227360713187	-29.85530625553334	5.86320142433481
C	33.79197910792591	-28.50999831384783	0.37799205352837
N	33.24144717884756	-25.55748793026335	4.87414286541944
N	34.72357002910727	-25.61037645704296	7.33461822865960
N	34.96336402461966	-27.51314897921297	3.80587593767702
C	32.93196249800847	-26.67775915534564	2.72327054984365
C	32.94529191657960	-24.02175291579519	6.76211589737237
C	36.45528661923171	-26.80562840583486	8.58243384438835
C	37.07640315630975	-28.69142122283735	4.17963013184569
C	30.60537155769303	-22.89182438276179	5.08267656711679
C	33.38939428027031	-22.95874017693438	9.63400070456904
C	38.89150398595210	-28.69499914597019	8.86892760008744
C	36.65400944538528	-29.74291182585032	1.30461990856516
C	32.56594643537748	-25.75562029015148	3.69887487208922
C	33.90019540883893	-24.55403653323404	7.62329316492540
C	36.93439168341875	-27.58348895191814	7.53499759718091
C	35.98419797431861	-28.32900452471050	3.40199710998606
C	31.46642151447695	-24.81452260802943	3.57552506789486
C	34.11473638195888	-24.10197047622474	8.98779981391998
C	38.10382782976027	-28.44287490796514	7.61727703262356
C	35.74188535286316	-28.81865736995459	2.05511986711544
C	31.50675303359372	-24.02667900316354	4.69629761189316
C	35.06939411014591	-24.92648827013835	9.52475114830002
C	38.31273955603641	-28.92634290066212	6.35371283789806
C	34.53489570118813	-28.30167229877329	1.66451697717775
C	32.61418387494921	-24.51443054193589	5.50294832170463
C	35.44673819672697	-25.85293342109557	8.47280887360661
C	37.24920868917202	-28.38419293638398	5.52267377692286
C	34.07168039421262	-27.47318320690897	2.76414096166612
N	36.43011007194072	-27.57582434249914	6.26018349314917
Fe	34.79273285375152	-26.63612871355575	5.59820824846925
C	32.80544112297298	-31.58049735429839	6.50250844102203
C	33.63506375113079	-32.18840615314620	7.62596495612732
C	32.41912348294498	-27.56154749575884	7.20602388147296
C	33.54995606273310	-27.98064229950982	6.31042892732319
C	33.74019743492074	-29.40489463159462	6.10774298222136
O	34.67959596405550	-29.96950146393375	5.56730007026690
O	32.69172421030053	-30.15815794264439	6.63289511460317
H	29.85950231162541	-22.68905563463585	4.30787249340043
H	31.16771026357867	-21.96305227767106	5.24752480177885
H	30.06012841977285	-23.10512798500028	6.01183646385355
H	31.03524750948475	-24.58021787332533	1.46719125099779
H	29.96174924267191	-25.70345911286194	2.30406829821059
H	29.77564186921583	-23.96327968429198	2.54062354525526
H	33.51898394993865	-27.55757301645373	-0.09516781926690
H	34.39251556628207	-29.07243269472601	-0.34381613641425
H	32.85997272560839	-29.06971357165633	0.53440782269380
H	36.30953672693698	-29.90005604182255	0.27768030838655
H	37.67798677853406	-29.35021968289555	1.25184682053588
H	36.71150648176759	-30.72833932384543	1.78560177486902
H	33.75061197072348	-22.77895041081857	10.65127221414874
H	32.30940722341570	-23.14764380432129	9.69871228401179
H	33.51846250842588	-22.02573938406536	9.06946688809864
H	36.74905750716932	-24.77182399304368	10.87836127568892
H	35.47465299868624	-25.85924394118861	11.43261458244548
H	39.73734083208203	-29.36378711856313	8.68228624680012
H	39.29602751205917	-27.76530559389796	9.29172522135379
H	38.27306647582175	-29.15901220800016	9.64884306983284
H	38.95760839487156	-30.80546680121034	5.51338303049909
H	39.93958129415676	-29.42140686568198	5.02240633579469
H	40.10593727369590	-30.08918373132744	6.65030478836104
H	35.23893561118040	-24.11076424964654	11.51447181145164

H	39.70978935629243	-22.76403193581931	4.17860313809078
H	38.61112887939213	-21.53725170413493	4.83460643722093
H	39.32901176015901	-22.74802636856387	5.90555622030222
H	33.21846530802502	-31.92354409312686	8.60196354251735
H	33.64943715532911	-33.28092986482471	7.54524647230381
H	34.66382835363859	-31.82766900482697	7.57584121174980
H	33.23994645025737	-31.82163363694999	5.53013570244301
H	31.77575745265627	-31.94558209971006	6.53448437452002
H	32.07877010941367	-26.54861197699776	7.00336718900576
H	31.56858291901526	-28.24131845643508	7.11742592596392
H	32.73276880375985	-27.58499611013397	8.26078641398804
H	37.16827610624294	-22.98740010224725	2.70658159943280
H	37.43786156346993	-24.75084122362647	6.51131321082793
H	35.32132031652511	-24.74259959247265	2.89914331938382
H	32.31112224200201	-26.73937849217714	1.83540557071430
H	36.94884010315934	-26.90299009507355	9.54388663590551
H	37.81220108590662	-29.34585202135548	3.72418053578308
H	32.36040039045484	-23.18643897487483	7.13334613803108

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B3LYP Scan/Melmid IPC Model/Triplet/200 degrees Constrained Optimization

C	38.91440483450305	-22.59607411423099	4.84057195394853
C	37.74877282360204	-23.51291744544254	4.66319963607370
C	37.18752115496827	-24.46289424915065	5.47778607551888
N	36.97355685262676	-23.54149402966880	3.51074537908335
C	36.00416167353326	-24.48096898492517	3.67262262332476
N	36.11017684780204	-25.05334722241145	4.85217595352045
C	30.51378934241876	-24.78672613566228	2.43991236608203
C	35.69068710678258	-24.88313335363560	10.91115435145432
C	39.42187475367930	-29.81982646696177	5.87460331068934
C	33.79118608965699	-28.53935509143106	0.41274354994155
N	33.24435714472337	-25.56904113644941	4.89798764458461
N	34.73970147911497	-25.60153805212331	7.35057296278280
N	34.97181937589873	-27.52528441650158	3.83251629517929
C	32.93488779519974	-26.69866828558401	2.75193320418338
C	32.94581277940383	-24.02878580880347	6.78127642199646
C	36.48992659953945	-26.77484224128096	8.59351631515183
C	37.09524317058361	-28.68685914205050	4.20056244425959
C	30.60107033526066	-22.91002197009665	5.10023860504575
C	33.39490011537134	-22.95234176156123	9.64664926452309
C	38.93981106627832	-28.64682698381039	8.87682841086145
C	36.65844299512511	-29.76263543662206	1.33494580386786
C	32.56808307647221	-25.77323959335730	3.72425627694770
C	33.90836353138695	-24.55137549365624	7.63967347310344
C	36.97059822714032	-27.55219267082411	7.54659711050539
C	35.99398804884368	-28.33966051777925	3.42824596103242
C	31.46594451595172	-24.83528742262164	3.59849205747049
C	34.12627772687974	-24.09212320859886	9.00119237738814
C	38.14588004857927	-28.40402580220407	7.62739340063852
C	35.74670767911321	-28.83783018334547	2.08539462608411
C	31.50450045296495	-24.04436093800012	4.71711740052627
C	35.09146985419122	-24.90568879817564	9.53597070737075
C	38.35078536292236	-28.89300595571487	6.36565270203694
C	34.53723950750214	-28.32475437727179	1.69650247649895
C	32.61397455733349	-24.52663295938969	5.52434905473849
C	35.47165801869435	-25.83247195673653	8.48553903708068
C	37.27882438280595	-28.36238721275948	5.53792004777083
C	34.07611736895146	-27.49194085334883	2.79351233235878
N	36.46025582138603	-27.55311245586602	6.27459664528800
Fe	34.80811072429263	-26.63440328389855	5.61977176216308
C	32.76023518322904	-31.57863770703065	6.31641276609258
C	33.40458919571878	-32.22855495045393	7.53391735469617
C	32.45232111858839	-27.57891853103608	7.24698804066528
C	33.57460850766860	-27.98716389023863	6.33576987159681
C	33.77117953783662	-29.40982263106249	6.12390121423889
O	34.77565069814464	-29.97699174643450	5.72238825879785
O	32.64615358688065	-30.15797126849847	6.46414644607885
H	29.85538168890795	-22.71007891306133	4.32450222749444

H 31.16202272943128	-21.98008663594410	5.26327233755913
H 30.05552102353669	-23.12182598817084	6.02956611399038
H 31.03463804649841	-24.60838784649762	1.48936699080857
H 29.96188256029807	-25.72968809265226	2.32976069508476
H 29.77455152199797	-23.98888101770283	2.56068265245530
H 33.51466238075056	-27.58904295051129	-0.06257642148214
H 34.39115215559417	-29.10241029096704	-0.30905380566531
H 32.86088275515756	-29.10073358195717	0.57327025701070
H 36.30843017141661	-29.92731047614571	0.31105354875517
H 37.68029461579452	-29.36572089778821	1.27357403286256
H 36.72353157137315	-30.74504423256661	1.82112341822184
H 33.75806233775035	-22.76735107410888	10.66228897858804
H 32.31644533608404	-23.14842945636005	9.71510811307740
H 33.51593394447505	-22.01998102728895	9.07925609379312
H 36.77663924015177	-24.72205927143891	10.87909416704173
H 35.52373622769182	-25.82995427004474	11.44182200961722
H 39.78682733981552	-29.31406638532876	8.68999037175889
H 39.34321915601852	-27.71382229937297	9.29339260541283
H 38.32585958461414	-29.10894588817910	9.66140144384090
H 38.99890599361630	-30.77266073363258	5.53011388373801
H 39.97466209098548	-29.38722632476564	5.03010496361540
H 40.14915706378342	-30.04841310216176	6.65992009584656
H 35.25967227730987	-24.08552139256846	11.52397560081155
H 39.69334036056122	-22.76684904071372	4.08530967507317
H 38.62163023785998	-21.53904853737803	4.78269921441963
H 39.36596053540695	-22.76053916676721	5.82313299202789
H 32.85480757199738	-31.97597849147503	8.44495820066935
H 33.40939255000755	-33.31902933944070	7.42822205491334
H 34.43636056950587	-31.89052610770246	7.64360706015760
H 33.33229561976422	-31.80409154474877	5.41383201620640
H 31.73252263626854	-31.92666365927877	6.18494257663408
H 32.08615930440984	-26.57597463663259	7.03627620214784
H 31.61549747148911	-28.27764523314095	7.18334139209729
H 32.78851026823494	-27.57776986775890	8.29508283049618
H 37.10608657099735	-22.96598930444818	2.69133654093403
H 37.48656950811996	-24.76139638710071	6.47155577852695
H 35.25852582472838	-24.71561328553101	2.92735833493459
H 32.31233669349596	-26.76557155256356	1.86563329484425
H 36.98876098586468	-26.86446138656147	9.55298348254540
H 37.83114726150544	-29.34148569790145	3.74555891323983
H 32.35722013217829	-23.19592396793347	7.15217879265282

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B3LYP Scan/Melmid IPC Model/Triplet/210 degrees Constrained Optimization

C 38.93220845828627	-22.60910185266932	4.74963265460608
C 37.74923241468492	-23.51074930934009	4.61570045050405
C 37.22008899422822	-24.47064954104088	5.44020883303852
N 36.91632206424180	-23.50997121764888	3.50400012535154
C 35.94687587889442	-24.44326022783758	3.69733492752037
N 36.10667057255194	-25.03912802235433	4.85909437623526
C 30.49096406192303	-24.85697593133154	2.48698826669166
C 35.75847660223452	-24.78625328061507	10.90685746309206
C 39.44794599881966	-29.80650123753632	5.92504811201133
C 33.79806532644376	-28.58513103651454	0.47013407612330
N 33.24436744003706	-25.58711270193102	4.93645376684527
N 34.76421423977964	-25.57479880075149	7.37290761899408
N 34.99025388680170	-27.53380418770236	3.87436090930364
C 32.93923439760381	-26.73390424691504	2.79882799548622
C 32.94217220886191	-24.03272610607149	6.80614760123508
C 36.53791456465629	-26.71497609622358	8.61440586495909
C 37.11782986533101	-28.68767390697545	4.24588872531286
C 30.56783356213981	-22.96087872861994	5.13371817336905
C 33.42288447233340	-22.90253040531818	9.64434579527685
C 38.98443925286806	-28.58877319101111	8.91255497018422
C 36.67231918401112	-29.79172051399984	1.39226452599840
C 32.56462034383325	-25.80810133716029	3.76766673687192
C 33.92419749503532	-24.52994964426031	7.65750660218370
C 37.01138514458695	-27.50829365063070	7.57642430775782

C	36.01339617933385	-28.34919383715701	3.47383558751451
C	31.44913094316524	-24.88564619944816	3.64133656764522
C	34.15644046563632	-24.04591542629426	9.00768015185557
C	38.18617157976204	-28.36063353603713	7.66317971355444
C	35.76164943122733	-28.86152296827878	2.13742354225070
C	31.48276249440097	-24.08720300375156	4.75452515420773
C	35.13877403592416	-24.83954897888895	9.54155881543169
C	38.38324204378120	-28.86817439680950	6.40784738627552
C	34.54874073252736	-28.35582181929420	1.74870951217966
C	32.60349615215304	-24.54907628524411	5.55869824297797
C	35.51355048062498	-25.77981131632313	8.50163599621967
C	37.30773655362175	-28.34692887008432	5.57824417057820
C	34.08886778274252	-27.51513140409905	2.83973649165676
N	36.49365286936599	-27.52689528052085	6.30763724402736
Fe	34.82994125891872	-26.62554861776513	5.65417308014864
C	32.68434677130564	-31.53911729748385	6.02690141537757
C	33.12065520435793	-32.30099127640319	7.27129375534983
C	32.53921837584535	-27.61386317659289	7.35244607572571
C	33.61645420172565	-27.99346712002796	6.37625830142065
C	33.79224619706712	-29.40998135742150	6.10346332115617
O	34.81938334800419	-29.99277239122294	5.79556785362703
O	32.60921484304889	-30.12665254543827	6.26053960119559
H	29.81570325553920	-22.77581440823443	4.36046440565054
H	31.11868093969015	-22.02312032187425	5.28631619422363
H	30.02985679029795	-23.17148763442536	6.06769768655707
H	31.00532624719183	-24.68142307721814	1.53239119599456
H	29.94845288748832	-25.80653445226151	2.38747545598651
H	29.74408463509342	-24.06576315282005	2.60446055936065
H	33.51896798564290	-27.64020224963514	-0.01430807897193
H	34.39589144352511	-29.15534184553118	-0.24779947991485
H	32.86884987731275	-29.14554982759907	0.64001713458756
H	36.31727901111417	-29.96869104634675	0.37216667082319
H	37.69261415108296	-29.39256041018605	1.32104438145436
H	36.74294033432701	-30.76856089479553	1.88880339809030
H	33.79825460207656	-22.69732937461865	10.65162564957703
H	32.34734857795336	-23.10729360632613	9.73101325464834
H	33.52740873781458	-21.97873535597274	9.05990754803913
H	36.84106442617859	-24.60841506159455	10.85559756192421
H	35.61483176376326	-25.72728766514026	11.45433403896719
H	39.83025793533930	-29.25887824504078	8.73074460516739
H	39.38989973755206	-27.65120292644687	9.31674681816793
H	38.37273843482502	-29.04114474546334	9.70455712623343
H	39.01844595111355	-30.76139129404588	5.59463772434779
H	40.00003240993232	-29.38800982389746	5.07300475423967
H	40.17680923718304	-30.02878382092176	6.71073560528281
H	35.32383362990127	-23.98629855984001	11.51400630871611
H	39.67087428762859	-22.77562953250842	3.95399149645934
H	38.64880309510510	-21.54831631717089	4.72329956613463
H	39.43025135440790	-22.79465076898144	5.70565470051974
H	32.45909033841875	-32.08133099740227	8.11392338453059
H	33.09319063169374	-33.38070508118346	7.08753449042062
H	34.14047414818953	-32.02694179357469	7.54686041828293
H	33.37000289949429	-31.73168164182768	5.19920649170856
H	31.67273706486476	-31.82459919520907	5.72743112818021
H	32.13498919741048	-26.61939947217268	7.16584536410313
H	31.71754112363885	-28.33301934171177	7.33463166460843
H	32.93770919841179	-27.60254498242098	8.37830512721962
H	37.01347106584824	-22.92070071616182	2.68942279401765
H	37.56687541357969	-24.79148529837280	6.41125492260273
H	35.16264881341445	-24.65789679398649	2.98648856544312
H	32.31298011249533	-26.81431869605852	1.91627425930027
H	37.04556373520090	-26.78726259952401	9.57071966274363
H	37.85151309844349	-29.34789428070122	3.79543825191103
H	32.34694003008659	-23.20327650474977	7.17417603333274

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B3LYP Scan/Melmid IPC Model/Triplet/220 degrees Constrained Optimization
 C 38.92499337234536 -22.59391832484166 4.71391260961393

C	37.74296891628375	-23.49942723978554	4.59909192284746
C	37.24049396151796	-24.47308272922682	5.42421597262648
N	36.87942219963260	-23.48620894314404	3.51119097615174
C	35.91896612884602	-24.42586808500942	3.71816991123942
N	36.11322433860610	-25.03764985476174	4.86637512526754
C	30.46740701756643	-24.94410006230620	2.52867825238451
C	35.84143036939380	-24.68856611235442	10.88365983253306
C	39.47367540967586	-29.81177884234499	5.96980846672636
C	33.82431974662953	-28.61857335532916	0.50489816531596
N	33.24842653889372	-25.61425779852500	4.96450983142482
N	34.79329043222531	-25.55727619889584	7.38422512829409
N	35.01300833794408	-27.55168421214601	3.90560786654725
C	32.95397371166566	-26.76996839545078	2.83027159012021
C	32.93523968430912	-24.05429582350621	6.82604325964374
C	36.59522318730124	-26.65948492704039	8.62142566898390
C	37.13598821043042	-28.71257572424526	4.28656773266207
C	30.51896258747628	-23.04372175641316	5.17320358647987
C	33.45299541309756	-22.86447856783430	9.63215092486547
C	39.04303338986967	-28.52837163434379	8.93478314068027
C	36.69546326782270	-29.82448408049222	1.43723766684427
C	32.56703267097538	-25.85038400194139	3.79982771599010
C	33.94187689897981	-24.52051807411042	7.66619679702101
C	37.05542724233292	-27.47679977061785	7.59648756605814
C	36.03477543646861	-28.37227067187262	3.51077622572569
C	31.43202061766236	-24.95075785724775	3.67798584660581
C	34.19150249508742	-24.00862285678959	9.00248771442198
C	38.23086140989349	-28.32819075821918	7.68956461384773
C	35.78420994365226	-28.89057285968861	2.17713686792562
C	31.45483368312191	-24.15116631552853	4.79010520520308
C	35.19615251594596	-24.77727710672970	9.53200216508078
C	38.41375678029409	-28.86373199086933	6.44408996650675
C	34.57254888393045	-28.38455521116229	1.78409579603445
C	32.59076283752725	-24.58814382139406	5.58781293798899
C	35.56422775053219	-25.73209464088572	8.50361400487624
C	37.33085312049356	-28.35729884895536	5.61415642777539
C	34.11116931386646	-27.53996563676165	2.87087570795472
N	36.52337526697714	-27.52258691342563	6.33418733120527
Fe	34.85320561295251	-26.62822196233593	5.67850128750166
C	32.54356499885981	-31.45043205643681	5.78430040950667
C	32.83919394042918	-32.28833582894680	7.02118687779439
C	32.65510891917317	-27.65267365487859	7.48933047202421
C	33.64298730099348	-27.99505796468240	6.41006383815591
C	33.76307296688981	-29.40115164292909	6.05567033666177
O	34.77757157474488	-30.02619216331187	5.79747765264512
O	32.53111154397395	-30.04571921678509	6.07620332239471
H	29.75783349255820	-22.87642379827350	4.40467663322177
H	31.05091992704573	-22.09414599613856	5.31989308288008
H	29.99215655188296	-23.26352048529235	6.11140348054720
H	30.97333994073393	-24.76199906514590	1.57078068805353
H	29.94276075117888	-25.90421392330627	2.43510529802094
H	29.70634640893368	-24.16673858398736	2.64755080266942
H	33.54623683244709	-27.67547589973872	0.01641337475915
H	34.42365928100989	-29.19142722783236	-0.20967551598563
H	32.89486819356750	-29.17851050673408	0.67499218393729
H	36.34133729883012	-30.00640906419554	0.41771490706425
H	37.71573426666765	-29.42547361170929	1.36496951669133
H	36.76581899003110	-30.79891586406723	1.93848720596017
H	33.84227812043048	-22.63744278324918	10.62941905029643
H	32.38194934103925	-23.08208389459076	9.74044167334247
H	33.53524309858842	-21.94940294326178	9.03073494947452
H	36.91878164026012	-24.48882048880246	10.80802657465513
H	35.72867017638707	-25.62326551041451	11.44886655590086
H	39.88711386332935	-29.20204663986638	8.75825206969704
H	39.45254838536826	-27.58196936599357	9.31360666016144
H	38.44053900369527	-28.96334614926358	9.74340804867697
H	39.04014270695523	-30.76964878844392	5.65369396747754
H	40.02391840752538	-29.40641296744574	5.11018337529639
H	40.20498539771585	-30.02576164975643	6.75557395370498

H	35.40163635278132	-23.88818447961042	11.48646828917540
H	39.64278908523335	-22.74518351824104	3.89641377274195
H	38.63589300181984	-21.53435413475194	4.71059274517689
H	39.44951008376417	-22.79062253592336	5.65341437058081
H	32.12727553561427	-32.06609457528333	7.82111747035992
H	32.76598530690228	-33.35583589662514	6.78586457910597
H	33.84801224224244	-32.08690970165661	7.38525788029818
H	33.27862921418651	-31.64844935095749	5.00141711194165
H	31.54349490491052	-31.66168962391683	5.39777448494636
H	32.20985476056551	-26.66516139903774	7.35808893831366
H	31.85013129016329	-28.38990953478736	7.53657048760731
H	33.14945458827334	-27.64358518598561	8.47236856007004
H	36.95185967097525	-22.88523092261750	2.70261210426831
H	37.61504278045823	-24.80554485996588	6.38093150312495
H	35.11608239463369	-24.63359358551008	3.02638126041734
H	32.32676237529007	-26.86037274343606	1.94940585654246
H	37.11614040728946	-26.70850286625530	9.57207976775173
H	37.86588427020043	-29.38065043654439	3.84163319391175
H	32.32948669622189	-23.23251103988128	7.19418806900356

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B3LYP Scan/Melmid IPC Model/Triplet/230 degrees Constrained Optimization

C	38.92381680390910	-22.58903664651697	4.66084481177359
C	37.73969644953971	-23.49440045685197	4.56920524033500
C	37.25241496126634	-24.46668462146325	5.40498436993644
N	36.85628514358909	-23.48270974252535	3.49737153662462
C	35.90004327778246	-24.42224893190843	3.72310798178056
N	36.11531469780623	-25.03232166181126	4.86851396854041
C	30.45060968549871	-24.99371775437297	2.57430962802910
C	35.90066353672783	-24.62540953410645	10.87830469800394
C	39.49041200345771	-29.81295291964928	5.99970721269182
C	33.81189015251251	-28.66133679702266	0.55303002045174
N	33.25508348253815	-25.62443426818779	4.99419843250187
N	34.81786231005503	-25.54048208344317	7.40123510659671
N	35.02096199162318	-27.56818758155401	3.93827106156805
C	32.95586511818623	-26.79418123559254	2.86782607764254
C	32.93780499760232	-24.06124840337550	6.85149128982796
C	36.64351633720617	-26.61396553604491	8.62918281881960
C	37.14128698252474	-28.73318241363402	4.32089902058557
C	30.49778873223137	-23.0842985554575	5.21215742160265
C	33.47466874663022	-22.84170378128012	9.64061528279669
C	39.09302577738108	-28.47880107976672	8.94659752929890
C	36.68035717921570	-29.87421530155678	1.48436174217393
C	32.56848355914772	-25.87240095958203	3.83501476029987
C	33.95788362180512	-24.51078402389003	7.68430231266478
C	37.09593688874914	-27.44292240239109	7.61032857516808
C	36.03702159015540	-28.39790518008404	3.54674438877681
C	31.42317857290713	-24.98517391818739	3.71691837153042
C	34.21789081900385	-23.98378662998098	9.01271937060595
C	38.27043980480586	-28.29532132910450	7.70567226348683
C	35.77718494950281	-28.92891107026696	2.21989804803691
C	31.44373884708576	-24.18223053545984	4.82653982863894
C	35.23828126056082	-24.73540487694362	9.53651067202614
C	38.43921616218761	-28.85231835861654	6.46790597476347
C	34.56662388556590	-28.41950259195610	1.82704102752917
C	32.58985147491492	-24.60397202733201	5.61814485302674
C	35.60383478303309	-25.69626223831650	8.51296447703946
C	37.35000563586561	-28.35549166452615	5.64027929115389
C	34.11389038320223	-27.56281697372464	2.90767679671664
N	36.55256819052488	-27.50560109490537	6.35367366313270
Fe	34.87401839266906	-26.62137591320326	5.70389086771323
C	32.56039878429009	-31.38587525345217	5.56048926564581
C	32.58446390548790	-32.26678336195928	6.80179444617397
C	32.69337636104019	-27.67750331949668	7.53227517352346
C	33.67920535902405	-27.99510139211358	6.44389366997849
C	33.80994854916516	-29.40119910142574	6.08011654486249
O	34.82887128093198	-30.05886289147238	5.97321911544158
O	32.56677229656558	-29.98916797770866	5.89311930451549

H	29.72948816238993	-22.92861639363268	4.44831778170187
H	31.01980812333983	-22.12813977510988	5.35172778929526
H	29.98010168165805	-23.30670207447150	6.15479546532821
H	30.94859975240854	-24.81592263124725	1.61147420679024
H	29.93159759340589	-25.95792321993620	2.49197717472580
H	29.68538838271413	-24.22032927293150	2.69245133539610
H	33.53859420374175	-27.72125011258755	0.05616366257325
H	34.40452097267545	-29.24548959970085	-0.15796357643728
H	32.87911368445128	-29.21286328966859	0.73211782007023
H	36.31864985353272	-30.06610818349152	0.46932863631648
H	37.70139634892367	-29.47946123690803	1.40067714358670
H	36.75128366697388	-30.84349645516403	1.99544388908935
H	33.87007314530705	-22.60460627976086	10.63312238733157
H	32.40645638635058	-23.06768763825243	9.75907552918802
H	33.54421268259907	-21.93003253814483	9.03244279659772
H	36.97258555839707	-24.40424161872636	10.78627742638232
H	35.81496977495560	-25.55875963804643	11.45037594887593
H	39.93778475502483	-29.15180229686466	8.77087718882862
H	39.50233949787474	-27.52692125456051	9.31161520293640
H	38.49816619597303	-28.90673732198795	9.76457856501847
H	39.04948002533934	-30.77420881130159	5.70481653264172
H	40.03405932088366	-29.42520948028411	5.12783565630146
H	40.22840834589105	-30.01661566631923	6.78197670221214
H	35.45309535155244	-23.83053008239202	11.48264839765737
H	39.62804049460473	-22.74407266672117	3.83232160091945
H	38.63514903018939	-21.52937035682562	4.65793852519650
H	39.46347888099714	-22.78233595928883	5.59242535738994
H	31.75467987323719	-32.02042772297269	7.47031855752288
H	32.49659661318211	-33.32265184161910	6.52295824468013
H	33.52168932688309	-32.13368862292351	7.34540785846411
H	33.41432076807752	-31.60514846618192	4.91630662742939
H	31.63778648123730	-31.53102155033166	4.99302334438875
H	32.22429638163285	-26.69940194037483	7.40803746456150
H	31.90237695694472	-28.43150316059268	7.57965950958741
H	33.19192213467509	-27.66229868490196	8.51330913446560
H	36.91404265058762	-22.88316804388500	2.68655288405704
H	37.64428247537659	-24.79804578387341	6.35509214303950
H	35.08488498839714	-24.63124736865955	3.04622785101422
H	32.32388812430010	-26.89255245354311	1.99123671498898
H	37.17431022014408	-26.64908887340879	9.57496575098578
H	37.86428078289224	-29.41216288708106	3.88125438391820
H	32.32616360980063	-23.24430044601523	7.22072577094980

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B3LYP Scan/Melmid IPC Model/Triplet/240 degrees Constrained Optimization

C	38.93646865463575	-22.60348419277779	4.63445277710634
C	37.74617544882244	-23.50160526439948	4.55184612517841
C	37.26107853143341	-24.47268366492526	5.39028634219814
N	36.85277343247461	-23.48254423735357	3.48846374786271
C	35.89278507816918	-24.41652887457559	3.72176138390983
N	36.11532982451849	-25.03016643217018	4.86381705789387
C	30.43955377678788	-24.99929554404648	2.58912497865243
C	35.92976153646605	-24.59077166698091	10.86690439135983
C	39.46676003029982	-29.84179217095928	6.01703830255738
C	33.79766543753284	-28.66547634252118	0.56476192396869
N	33.25118565049390	-25.62096709226562	5.00335042210468
N	34.82331380013724	-25.52838361186879	7.40314434839526
N	35.01343112159776	-27.57230905475632	3.94751349364554
C	32.95018967273166	-26.79211200706696	2.87773156401197
C	32.93316418482535	-24.05915771885254	6.86092479600983
C	36.65660678927406	-26.59451376689950	8.62674938214264
C	37.12523121607221	-28.75174895252959	4.33433909476120
C	30.48142093732297	-23.09525713364258	5.23102827866068
C	33.48798737516480	-22.82224046867771	9.63859121693085
C	39.09181891995565	-28.47648031776891	8.95233391166762
C	36.65755386551788	-29.89569331457716	1.49928047273614
C	32.56311812028243	-25.87105655735925	3.84555755607312
C	33.96177872590191	-24.50025116027405	7.68770079664564

C	37.10011940453859	-27.43423966892233	7.61282212742567
C	36.02399666824048	-28.41027252325444	3.55817606143216
C	31.41358793202491	-24.98846616573574	3.73046890019159
C	34.23018055328643	-23.96527014672641	9.01113109591074
C	38.26782598656590	-28.29570549754423	7.71199792833607
C	35.76051134984034	-28.94295672422506	2.23291872793000
C	31.43194679157600	-24.18780265048944	4.84152489485937
C	35.25747015627105	-24.71037055197970	9.53085355336113
C	38.42725654652365	-28.86567888940687	6.47914001893891
C	34.55354387752259	-28.42565585455456	1.83848605413390
C	32.58213783678695	-24.60513472384385	5.62993217972304
C	35.61762161932496	-25.67611631566176	8.51016295626047
C	37.34009272837599	-28.36587620570370	5.65041679305108
C	34.10606872679676	-27.56408831487170	2.91715241517556
N	36.55219808374254	-27.50277403414959	6.35857037579531
Fe	34.87393000117394	-26.61453594705646	5.70972996904563
C	32.58778690979018	-31.35718525072089	5.46391088152130
C	32.53613922963608	-32.23168745027028	6.70893816480601
C	32.75648192145763	-27.70768433247386	7.60174776434317
C	33.68406157372438	-27.99047801895700	6.45419215828848
C	33.82586374303831	-29.39860580899200	6.08816500594348
O	34.83548582942122	-30.07655309293184	6.08134863441716
O	32.59506798322490	-29.95630520330652	5.78633121983895
H	29.70945347407939	-22.94351869901610	4.47008512912750
H	30.99866047799864	-22.13623923038540	5.36898469271016
H	29.96861182971854	-23.32092490394495	6.17553554504862
H	30.93510762091134	-24.81488594769169	1.62623847145065
H	29.92664018074580	-25.96649371352834	2.50402635436652
H	29.66963079900080	-24.23115897932945	2.71097566729081
H	33.53071294321077	-27.72472433853320	0.06574197948315
H	34.38672994845980	-29.25500736746677	-0.14475042280121
H	32.86122133088530	-29.21042263568938	0.74476521599105
H	36.29445732705960	-30.08748740007985	0.48473282409268
H	37.68105378250021	-29.50763290181585	1.41450653578769
H	36.72271238347490	-30.86443551066712	2.01220972258931
H	33.89101977048423	-22.57772280982125	10.62622059193608
H	32.42169434187571	-23.05147340635996	9.76771497582774
H	33.54880276049158	-21.91403731323913	9.02436201962697
H	37.00134166672563	-24.37231824097096	10.76539340520749
H	35.84657435167402	-25.51926764220682	11.44725798907238
H	39.93230497837420	-29.15541329106657	8.77899247702285
H	39.50739316849634	-27.52487198299824	9.31094631509871
H	38.49608147642911	-28.89620355885442	9.77393700759111
H	39.01475970842326	-30.80193489292155	5.73551295190681
H	40.01024217743806	-29.46986589838068	5.13821293176529
H	40.20637519102613	-30.04374264214730	6.79823467328332
H	35.48783442697931	-23.79026127005385	11.46796119289778
H	39.63146014835346	-22.76004679190788	3.79846361023807
H	38.65412877114725	-21.54211793701647	4.63790567835287
H	39.48424467364898	-22.80310841959310	5.55995389610955
H	31.67385650651280	-31.97426808074404	7.33061765775013
H	32.45290230069589	-33.28782287187468	6.42999440445421
H	33.44411660945178	-32.10503165525135	7.30079363405814
H	33.47057166844360	-31.59125897533515	4.86546605011453
H	31.69435581784880	-31.49259415528764	4.84976202655877
H	32.28718643198457	-26.72393548496328	7.53474109110447
H	31.96176044828932	-28.45905515183359	7.65896054243372
H	33.29991158276223	-27.73338216200738	8.55876056605250
H	36.90653449251595	-22.88177947148849	2.67827803489638
H	37.65972089228316	-24.80803299671823	6.33616177784698
H	35.06971449350132	-24.61910054677166	3.05254554318939
H	32.31703993863077	-26.89040304676920	2.00195667055803
H	37.19196276331114	-26.62424353453180	9.57015561701719
H	37.84189863084136	-29.43959534663872	3.89812094527286
H	32.31950711501217	-23.24455196807183	7.23200746241667

C	38.92722663375414	-22.59410445032375	4.60276173795782
C	37.73767914012209	-23.49384376566551	4.52765567636074
C	37.24724134244781	-24.45081425917965	5.37913261185770
N	36.85196248870646	-23.49381796355361	3.45767845172623
C	35.89172399561275	-24.42539072727142	3.69937438638298
N	36.10645729282795	-25.01898433267215	4.85346019270711
C	30.44425034430100	-24.94266669681076	2.59778796413246
C	35.93085145547177	-24.59713946213659	10.88106737014915
C	39.42143016114490	-29.87534195735766	6.02043980381122
C	33.73087548759246	-28.67968616943383	0.59303504377126
N	33.24597181805957	-25.59673244239081	5.01532383106736
N	34.82129006106308	-25.51521575976673	7.41269262338728
N	34.98560725403835	-27.57046816431970	3.95627077569567
C	32.92890902333598	-26.76903482954594	2.89145437846423
C	32.93650496635841	-24.03744739080933	6.87723307818288
C	36.65993596632543	-26.58286087278212	8.62461092674045
C	37.08234609056620	-28.77512820285447	4.34327713844517
C	30.50242096092650	-23.04232627660101	5.24155699408713
C	33.48499624480037	-22.82456386392833	9.66657203881594
C	39.08078595817143	-28.48052416795210	8.94485062262516
C	36.57562156356976	-29.94790441215872	1.52294993827283
C	32.55587813480145	-25.83942405299304	3.85664678974397
C	33.96012785080017	-24.48899733806429	7.70395762634962
C	37.09845706738309	-27.42056248630103	7.60689842596314
C	35.97965984100117	-28.42930077449363	3.57001286180684
C	31.41707142318553	-24.94390836089216	3.74025535654583
C	34.22860716214674	-23.96231797525306	9.03142252805135
C	38.25610029768362	-28.29446232692960	7.70590183897194
C	35.69870520961107	-28.97317773780396	2.25218533500894
C	31.44198340898044	-24.14463053366239	4.85259946508049
C	35.25731530337016	-24.70876720394853	9.54505935449975
C	38.40140167720824	-28.87665802170110	6.47719627912802
C	34.49883465510672	-28.43907435267527	1.85934668407911
C	32.58585856379746	-24.57494231257230	5.64222986727451
C	35.61762249146040	-25.66783572438124	8.51734152377965
C	37.31680584354655	-28.36935816235140	5.65043407725159
C	34.07244877947827	-27.55879891610882	2.93187779000699
N	36.54662591215288	-27.48667645441625	6.35444040392572
Fe	34.86773952895871	-26.59598763496520	5.71577122625967
C	32.92502282471783	-31.42153312396205	5.40159930275081
C	32.55566883824290	-32.23826515974975	6.63147098272155
C	32.678066537396457	-27.70223814679392	7.52823648877845
C	33.70016984142375	-27.98606430197720	6.46521451642084
C	33.95150287414088	-29.40849435910233	6.20966913044228
O	34.94643029487938	-30.05462294906799	6.47165810294671
O	32.84086653490143	-30.00672136017391	5.64972583192219
H	29.73268799629207	-22.88240799604925	4.48004548425208
H	31.02950974099246	-22.08880784526905	5.38022923614425
H	29.98628212537553	-23.26269527011623	6.18550341591888
H	30.94383293425887	-24.76913076910215	1.63502302033367
H	29.91573374995501	-25.90167523463298	2.51482461700071
H	29.68655800796751	-24.16193420250538	2.71629209708927
H	33.47575452382080	-27.73980865188346	0.08619509800738
H	34.30579442329203	-29.28557784166115	-0.11428109892800
H	32.78686278311298	-29.20728518614370	0.78467157617404
H	36.20180933291919	-30.14550793845259	0.51338895189132
H	37.60422052252763	-29.57651168318257	1.42583959110197
H	36.63089117353581	-30.91224298593936	2.04545325069236
H	35.88348756963119	-22.59037705579229	10.65853686216083
H	32.41773609879201	-23.05343203026752	9.78791924945483
H	33.55021558765251	-21.91028874585746	9.06174960602553
H	36.99984116586168	-24.36577513235869	10.78021265605949
H	35.85885246884725	-25.53322648164947	11.45050800680730
H	39.91836142756559	-29.16248943163171	8.76945690412802
H	39.50034009998827	-27.53128265282288	9.30491925215203
H	38.48377283813716	-28.89988250083647	9.76569213895452
H	38.95157501001822	-30.83313206594841	5.76074832442088
H	39.96146515981012	-29.52721953533753	5.12986042343754

H	40.16578332125069	-30.07555822404959	6.79753445175900
H	35.48136598652645	-23.80848945241404	11.49215157794093
H	39.62894106698779	-22.76676008303322	3.77560495116853
H	38.64503948178513	-21.53287529139831	4.58351248290715
H	39.46740739717440	-22.77595668119266	5.53634317398810
H	31.56047721945307	-31.96701899480422	6.99465274122132
H	32.55206936144992	-33.30744349518537	6.39317975165595
H	33.27772124668925	-32.07048055130396	7.43261493165757
H	33.93421286627122	-31.66515281386180	5.06434260806663
H	32.22201225440570	-31.59858313611900	4.58429724567670
H	32.20912814031773	-26.72320895331990	7.41387026446876
H	31.88470588830287	-28.45956135236990	7.51805960130876
H	33.13071250211260	-27.72173255156198	8.53255213011866
H	36.91104099916502	-22.90674768673141	2.63788542426881
H	37.63956786168978	-24.77038249798682	6.33309903581835
H	35.07403040143556	-24.64047024233305	3.02744858949823
H	32.29176093016809	-26.86204546336890	2.01795057749057
H	37.19824112128508	-26.61707054366813	9.56614842686521
H	37.78524644899128	-29.48013386658352	3.91199753948740
H	32.32670976704346	-23.22115703641965	7.25089215700359

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B3LYP Scan/Melmid IPC Model/Triplet/260 degrees Constrained Optimization

C	38.93606306315048	-22.61844224214633	4.56965148832601
C	37.73946200865456	-23.51011659496125	4.51185168276346
C	37.25599495647749	-24.46504689660473	5.36961473772623
N	36.83725201577658	-23.50272616116259	3.45580704853905
C	35.87438753632418	-24.42789754181873	3.71152674154650
N	36.10311096767851	-25.02460903455490	4.86127063062069
C	30.41787435885605	-24.99148241523232	2.63058057686820
C	35.98087870146393	-24.50890379743898	10.85985472431509
C	39.40634337371566	-29.89493396590279	6.07573932385899
C	33.72725002177457	-28.70865470542789	0.63032862310070
N	33.23749139486899	-25.60587346063877	5.03802355439536
N	34.82574115304332	-25.49629700096327	7.42532990849570
N	34.98059766541309	-27.58517239708290	3.98903316882265
C	32.92335210811218	-26.78942631884035	2.92026783735080
C	32.92382401122593	-24.03935675965556	6.89200596831680
C	36.67986899895907	-26.53991380688624	8.63627123010395
C	37.06924894288079	-28.80135912421627	4.38879327140915
C	30.46348613256542	-23.08506389141024	5.27037437959002
C	33.50592334504046	-22.77350145624178	9.65058966049418
C	39.09419066111815	-28.44288115877375	8.97516236534030
C	36.56511009462695	-29.98362745129488	1.57270759519662
C	32.54522560555343	-25.86005214667864	3.88327923226041
C	33.96231467051755	-24.47017132760052	7.71134789613655
C	37.10585136622861	-27.40000022880697	7.63206518828924
C	35.97122468576749	-28.45192442292329	3.61021724051602
C	31.39521961482394	-24.97794779628656	3.76908130043033
C	34.24620574410959	-23.91898650740089	9.02530351033266
C	38.26065762010602	-28.27715950108315	7.73920517894992
C	35.69044291435480	-29.00176061390063	2.29523948584342
C	31.41482631978500	-24.17641140779190	4.87944439113231
C	35.28694171614457	-24.65024188367712	9.53707130700660
C	38.39407192828584	-28.88320165515487	6.52089515302445
C	34.49350752950649	-28.46426996770823	1.89701696723194
C	32.56826380939216	-24.59057182660106	5.66464250456271
C	35.63697220275873	-25.62631256284620	8.52227083814147
C	37.30695420379683	-28.38427839086739	5.69176762780454
C	34.06847363829202	-27.57693295286639	2.96378702285468
N	36.54378849390712	-27.48716975857236	6.38547758885712
Fe	34.86520321168321	-26.59436152094308	5.73989979160980
C	32.94431494257284	-31.33983465659854	5.19139810183849
C	32.47687528414489	-32.22160046635076	6.34017567229433
C	32.76906172993591	-27.73878965190435	7.65289808525098
C	33.69965544263398	-27.98261786312194	6.50004217761846
C	33.93588677910865	-29.40250235812164	6.19599038937282
O	34.88959907759918	-30.08458595533177	6.50968925299927

O	32.86479298681487	-29.93924235719927	5.51823016168789
H	29.68693239653665	-22.93796729598971	4.51318790022020
H	30.97894936390225	-22.12420470398542	5.40220799516923
H	29.95652864499450	-23.30880592803523	6.21847253191431
H	30.91146819085636	-24.81486222158550	1.66526347309025
H	29.90050176177930	-25.95693714296685	2.55254890265548
H	29.65162518282907	-24.21928211735029	2.74999467291925
H	33.47881360778612	-27.77063214815490	0.11680749587514
H	34.30034382695239	-29.32244807499204	-0.07163164537724
H	32.77969929561462	-29.22945930638928	0.82301319600552
H	36.19129014862757	-30.18676910195504	0.56427276812541
H	37.59466047885065	-29.61539004435162	1.47366464705613
H	36.61797923626592	-30.94476165740188	2.10133636831557
H	33.91816786177901	-22.51899401546438	10.63188042829121
H	32.44193053845618	-23.00568467917119	9.79257578752181
H	33.55687173797332	-21.87031496621928	9.02806934220677
H	37.04665432776846	-24.27320565234429	10.73739281114442
H	35.92392557569959	-25.43386535816294	11.44888052725825
H	39.92811055108680	-29.13087481872219	8.80600037142124
H	39.51976753617747	-27.48847454766667	9.31399589534778
H	38.50251986966627	-28.84470656318701	9.80853190543858
H	38.93011081655008	-30.85423797552441	5.83388422868849
H	39.94439505451864	-29.56470222466196	5.17714599806237
H	40.15324217809915	-30.08654725871241	6.85259794934301
H	35.53622877026194	-23.71106315149756	11.46248272095016
H	39.62390437264251	-22.79496915282554	3.73173403946026
H	38.66077994278150	-21.55531477990041	4.55574809105563
H	39.48916857887482	-22.80496617615774	5.49470204213770
H	31.46269490749517	-31.95348031594311	6.64901683791391
H	32.47374134852431	-33.27390297606987	6.03600516566000
H	33.14309753007965	-32.11692440045276	7.19821902545028
H	33.97116109698439	-31.58110210214376	4.91071781802491
H	32.29817062838201	-31.45318035893514	4.31801581684200
H	32.31764600415993	-26.74524200237954	7.62572963927616
H	31.95555664623530	-28.47642338590343	7.66021327990514
H	33.29057005265669	-27.82784733714011	8.61978364122287
H	36.88756640719523	-22.91497225750215	2.63592527417573
H	37.66063654959316	-24.78813682668449	6.31721685784799
H	35.04486581642812	-24.63649024295238	3.05218412789109
H	32.28576872471860	-26.88893818479476	2.04781315323587
H	37.22765306391673	-26.55596531936415	9.57283612448249
H	37.76770763909271	-29.51466518451178	3.96396521478806
H	32.30962769265626	-23.22541017325481	7.26364069578955

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B3LYP Scan/Melmid IPC Model/Triplet/270 degrees Constrained Optimization

C	38.91819051975561	-22.59783010240639	4.58787636864469
C	37.73175788958065	-23.50173936790903	4.51315962060957
C	37.23224377212640	-24.44477070670905	5.37487039485460
N	36.85986276998920	-23.52228078991245	3.43203550654467
C	35.89797239904416	-24.45102241161299	3.67793662143327
N	36.09871518310385	-25.02375409461889	4.84500221435261
C	30.42887547057869	-24.90527423603060	2.61527414402909
C	35.95792406591839	-24.56528757242690	10.87284597347983
C	39.36021251913695	-29.92532667800742	6.03874459281802
C	33.65904261582276	-28.69238464951693	0.62095210154722
N	33.23244778859661	-25.57372881693136	5.02666832009896
N	34.81973183841503	-25.49301329024232	7.41586486376345
N	34.94664956108502	-27.57416685175119	3.96879985523683
C	32.90138793053318	-26.74617498301826	2.90429573946541
C	32.93085953273698	-24.01700124994178	6.89212136879155
C	36.66853659744834	-26.55605198394092	8.61642355561874
C	37.01274068675441	-28.82690981108940	4.36837774245534
C	30.49333669071821	-23.01577438079996	5.26679562825157
C	33.49485067792957	-22.80299263566052	9.67786697469543
C	39.07480774133629	-28.46872963382980	8.93776072249220
C	36.47414514826565	-30.01859092142982	1.56092337597989
C	32.53914221297597	-25.81199945265754	3.86896370278964

C	33.95958927310377	-24.46770542716166	7.71270426823374
C	37.08947002015941	-27.40954448363729	7.60472594143211
C	35.91631720741580	-28.46399838432002	3.59269916680203
C	31.40337519315237	-24.91224272905484	3.75626717061008
C	34.23756406232060	-23.93834507875897	9.03745556994917
C	38.23742459335860	-28.29514225730425	7.70562179812559
C	35.62021932897462	-29.01723973478300	2.28153990242421
C	31.43120379289353	-24.11726074115150	4.87154886829946
C	35.27327401154825	-24.68020328849468	9.54280633473527
C	38.35793504065247	-28.90531664332416	6.48788879627083
C	34.43410779973926	-28.45743532619440	1.88401379816958
C	32.57590963973159	-24.55202623046367	5.65739516328120
C	35.62597053631554	-25.64124347373232	8.51396922135483
C	37.26979493428792	-28.39948124358848	5.66493516672527
C	34.03108304279526	-27.55518694581000	2.94795721590374
N	36.52133035698196	-27.49068663815422	6.36040987038026
Fe	34.84945968775495	-26.58052612602297	5.72302786744652
C	33.32987250588923	-31.44515357733961	5.31720194772733
C	32.57384270462841	-32.23811946529644	6.37292539309865
C	32.67113077947539	-27.69212311673304	7.56207848955951
C	33.68478849695787	-27.96767004917739	6.48765575316852
C	34.02337215897930	-29.39731845511451	6.35024750988799
O	34.90242648082315	-30.00563751483981	6.92393374761042
O	33.15569635326850	-30.02535507170336	5.49146402711063
H	29.72105847122557	-22.85356481810895	4.50837438655297
H	31.02096800081459	-22.06273697650548	5.40658513365963
H	29.98041334818353	-23.23906377306426	6.21180504265560
H	30.92742245003886	-24.72922574199533	1.65242772553047
H	29.89851358595899	-25.86304631673230	2.52959252099651
H	29.67270052900162	-24.12365650937767	2.73753859337401
H	33.42829366432757	-27.75206656074947	0.10328549423553
H	34.21730069525632	-29.32122695120812	-0.07964333351020
H	32.70157957006710	-29.19240593509750	0.81938278471542
H	36.09207726855671	-30.22093449806522	0.55538715191673
H	37.50955094866980	-29.66905973363211	1.45463352304914
H	36.51307695487080	-30.97775849052185	2.09439077913691
H	33.89895172059563	-22.56831124452055	10.66744624508416
H	32.42909961556854	-23.03526958311328	9.80584703347133
H	33.55339843249412	-21.88810359403129	9.07328251163045
H	37.02500230719500	-24.32918639770760	10.76284997726807
H	35.89495458497746	-25.50170131113748	11.44276492519781
H	39.91030206801970	-29.15288605878481	8.76095281077678
H	39.49817468110461	-27.51604452970125	9.28375874955691
H	38.48538421204606	-28.87966112915216	9.76823612439445
H	38.87816832571905	-30.88529251338893	5.81096215782726
H	39.88852835831094	-29.60478858248116	5.13097763064125
H	40.11556234153341	-30.11347446029310	6.80818751451935
H	35.51017932730475	-23.77859254711871	11.48772362806406
H	39.63086004704957	-22.78276874968760	3.77285235008747
H	38.63372811842290	-21.53780675444752	4.54675559679376
H	39.44673338778741	-22.76207973402341	5.53132811877232
H	31.51554553172527	-31.96300274534080	6.38142866672215
H	32.64551005916140	-33.31202703519751	6.16987297304438
H	32.99101056086481	-32.05071857862088	7.36420013761472
H	34.39562072726691	-31.67900024806667	5.34457653325534
H	32.94290767439045	-31.64848508106613	4.31624679505713
H	32.20974639695687	-26.70867189451154	7.46097851858298
H	31.86697792387150	-28.44112984907250	7.53922682459165
H	33.11938817636913	-27.73816792922289	8.56813479335245
H	36.92790349056650	-22.94893464077794	2.60328998185394
H	37.61290565924803	-24.74674029962557	6.33924493434009
H	35.08862339376866	-24.67849165597330	2.99997530590251
H	32.26094937114888	-26.83417210923283	2.03263159312362
H	37.21639491356225	-26.58399433482030	9.55258447970444
H	37.69788442938775	-29.55336876922674	3.94391838480434
H	32.32287404855040	-23.20095080499353	7.26923622539255

B3LYP Scan/Melmid IPC Model/Triplet/280 degrees Constrained Optimization

C	38.92615893655410	-22.63399152885653	4.56899097250576
C	37.73298452420026	-23.52947137947497	4.50055839635923
C	37.22261149049295	-24.45778581147442	5.37183009632285
N	36.86590486075013	-23.55727186795254	3.41571715748106
C	35.89612164442881	-24.47571373266726	3.66861142653852
N	36.08733139103430	-25.03502007711660	4.84381030609880
C	30.41076272446794	-24.86800651693837	2.63235681023638
C	35.96841655735994	-24.55161536582612	10.87150653142193
C	39.30025004584100	-29.96727066178881	6.05072601670250
C	33.59198870303229	-28.70060842679822	0.64548393560417
N	33.21676330205377	-25.55342653744095	5.03598765201336
N	34.81047679020266	-25.47942645062290	7.42088464456335
N	34.90819951487055	-27.57174644809720	3.97873424104468
C	32.86770296732220	-26.72926244512189	2.91805729366422
C	32.93252755218423	-23.98988724914739	6.89924104959435
C	36.65572526957050	-26.55280123624960	8.61797903355918
C	36.95635543223653	-28.85273520840245	4.38174827184122
C	30.49863689688198	-22.97348224986047	5.27968286978298
C	33.51214253745141	-22.77556800885378	9.68201961776659
C	39.04182463627016	-28.48998476059300	8.94117970645931
C	36.39637084878851	-30.05248790447978	1.58336915503088
C	32.51766971485845	-25.78856978640912	3.88089774575508
C	33.95922108387396	-24.44730785389529	7.71849975362404
C	37.06379665706265	-27.41627051579461	7.60966546812216
C	35.86346077842882	-28.47752136638207	3.60652492538611
C	31.38917817379543	-24.87997283661861	3.76993650884638
C	34.24551239789207	-23.91680239265981	9.04131223124551
C	38.20174923707087	-28.31409461078549	7.71128838946111
C	35.55624489655160	-29.03659805074673	2.30003037199201
C	31.42696073818826	-24.08271804692195	4.88345851621623
C	35.27807238010899	-24.66428126971817	9.54422909089564
C	38.31008967313746	-28.93408851466549	6.49702185662709
C	34.37576793436793	-28.46535127949474	1.90305530280457
C	32.57051347795220	-24.52458328428784	5.66647198379535
C	35.61983661766901	-25.63060556944548	8.51626151009947
C	37.22459410083711	-28.42121196259171	5.67521747711254
C	33.98865049279439	-27.55001592177249	2.96219890348094
N	36.48952797599514	-27.49903366463930	6.36804385988629
Fe	34.82538944921072	-26.57143669902388	5.72990377743446
C	33.65069828928843	-31.43663926204236	5.29311121661950
C	32.75265746914214	-32.27211425045877	6.19349659536665
C	32.61523011221911	-27.65671962322007	7.55169653891735
C	33.66021309334784	-27.95075889472628	6.51211879744519
C	34.03675686892674	-29.37735440025598	6.44854716630132
O	34.80098127670327	-29.95930002129693	7.19062375578962
O	33.38149770886780	-30.02782227257391	5.43637738688567
H	29.72440979383526	-22.80783105837064	4.52405222883968
H	31.03354623805280	-22.02385366055983	5.41478181476422
H	29.98812154890242	-23.19079749290805	6.22736060275450
H	30.90698193656751	-24.69611362049656	1.66757288962572
H	29.87406788443158	-25.82250991774969	2.54961421578214
H	29.65987118669723	-24.08161162363006	2.75644177434964
H	33.37131541749451	-27.76189937064573	0.12051169549669
H	34.13855465653634	-29.34299603811796	-0.05202529731257
H	32.62889588253692	-29.18591119908887	0.85292370107348
H	36.00498804042518	-30.26197741142517	0.58288290988655
H	37.43384416499559	-29.71276561702410	1.46550116043039
H	36.43181952471247	-31.00644459478769	2.12635715153901
H	33.92341879030182	-22.53931122317841	10.66826740311296
H	32.44612819256307	-23.00247562653930	9.81730319187218
H	33.57126026882665	-21.86313524503396	9.07380090144588
H	37.03772840719618	-24.32817944768490	10.75695587736143
H	35.89673363134158	-25.48489738656829	11.44551136432377
H	39.87187522692012	-29.18064650882741	8.76401392347860
H	39.47313082321671	-27.53930691586648	9.28276064971126
H	38.45173339738623	-28.89417906797701	9.77440701400707
H	38.80862409791987	-30.92406733470431	5.82988823479492

H	39.82942140607397	-29.65779985364659	5.13961867334520
H	40.05574971651120	-30.15857775222641	6.81918955155066
H	35.53164592398682	-23.75731003772028	11.48451516793380
H	39.64061872992865	-22.83492836748496	3.75935842974034
H	38.65029541586200	-21.57236535875087	4.51331943000384
H	39.44947388759309	-22.79050260274416	5.51665573431033
H	31.69862191468237	-32.05222592038533	6.00296016670227
H	32.91683499851001	-33.34015869149123	6.01454339639313
H	32.96706892353331	-32.06584004028144	7.24365120399710
H	34.70390486070910	-31.62081137303741	5.51230728654451
H	33.46216252567540	-31.64531036446077	4.23778359478596
H	32.16756089833176	-26.67012744920741	7.42730608838585
H	31.80303343823756	-28.39693125796746	7.50840659393518
H	33.02787278570609	-27.70112504850361	8.57303861884393
H	36.94183828753145	-22.99478164846744	2.58025570239613
H	37.59658156515025	-24.75031460728231	6.34170469581200
H	35.08838948589336	-24.70604711719708	2.98972080078135
H	32.22312137905336	-26.81442670555017	2.04915501486420
H	37.20713699924580	-26.58116943705489	9.55200549531364
H	37.63107760458900	-29.58956887826335	3.95832600976648
H	32.33182990305010	-23.16836700190250	7.27609432255484

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B3LYP Scan/Melmid IPC Model/Triplet/290 degrees Constrained Optimization

C	38.92240739591352	-22.66395757669732	4.54250798081417
C	37.72244358636359	-23.55121686801934	4.48660858523031
C	37.21654799314756	-24.47809751071523	5.36198451578293
N	36.84224109915786	-23.57106827243000	3.41223219838540
C	35.86946043096820	-24.48354529449895	3.67488414304801
N	36.07119757104193	-25.04670975908092	4.84651274971263
C	30.38530176258884	-24.88961082305189	2.65352666363737
C	35.99693422415650	-24.50046610007917	10.85447826364694
C	39.26645041451467	-29.99750478693122	6.08516932955364
C	33.58179664151537	-28.70617472151029	0.66114240344237
N	33.19860546514207	-25.56373252125722	5.05209331480869
N	34.80807009439348	-25.46851538426781	7.42543360591946
N	34.89197495668635	-27.57966034802202	3.99733498358820
C	32.84796443495520	-26.74406829908121	2.93767654612646
C	32.92809861003631	-23.98229015504723	6.90190762864538
C	36.65086308211763	-26.54174670690574	8.62720753092385
C	36.93740055179657	-28.86536529188934	4.40369868149559
C	30.48202539027102	-22.98145642771410	5.29073220139197
C	33.54040454989949	-22.72795511051695	9.65954193594770
C	39.01715750050686	-28.50158916954887	8.96693675266805
C	36.38900651029734	-30.05268580318661	1.59992450975404
C	32.49623870357188	-25.80389220751917	3.90017394631115
C	33.96344329557279	-24.42908289208151	7.71627490244919
C	37.04821422773878	-27.42051043084477	7.62783282118260
C	35.84894085671032	-28.48378235055263	3.62545523134735
C	31.36656095506683	-24.89650784104138	3.78868052754688
C	34.26296514253318	-23.88184485550368	9.02908236031845
C	38.17896579700628	-28.32692289863975	7.73561764649318
C	35.54499252811034	-29.04059798999209	2.31747819044233
C	31.40818379209909	-24.09362475341323	4.89776058106223
C	35.29547788315900	-24.62812537160208	9.53434990542859
C	38.28358941498226	-28.95458866002696	6.52487333212520
C	34.36333994017462	-28.47174683898112	1.92030141441213
C	32.55533578497701	-24.53075108818378	5.67860343935615
C	35.62369167646049	-25.61054935508717	8.51742890923221
C	37.20298833343391	-28.43755210535965	5.69905164997058
C	33.97285732763336	-27.55948740511451	2.98057703820353
N	36.47252773509200	-27.50806323622591	6.38699986992801
Fe	34.81023933752839	-26.57672874829084	5.74413905285262
C	33.74355800461506	-31.38744353239807	5.19235955784343
C	32.78028298204712	-32.26200831758698	5.98143135472535
C	32.69172575210312	-27.65622964442887	7.67134865362997
C	33.65755517763345	-27.95297458904692	6.55711879066844
C	34.01392525061365	-29.38265945840188	6.46601225634040

O	34.69397244982095	-30.00281347041454	7.25903170545943
O	33.45854172203916	-29.98620665572142	5.37139796063686
H	29.70447220836453	-22.82060381356813	4.53748682702206
H	31.01786997018236	-22.03109626683856	5.41684130604959
H	29.97586194557824	-23.19211263224745	6.24220567942042
H	30.87908589784096	-24.72087536756330	1.68690859760145
H	29.84917379879448	-25.84480377739439	2.57556138450243
H	29.63417779601294	-24.10326142546253	2.77647455758200
H	33.36106536411457	-27.76701644260523	0.13700324173334
H	34.13012099333041	-29.34710879474406	-0.03632635962289
H	32.61887057575214	-29.19268357751318	0.86641984338161
H	35.99727344081483	-30.26443984961909	0.60006772870936
H	37.42466508852303	-29.70794304359037	1.48060759786881
H	36.42990804797290	-31.00624211709754	2.14326493023864
H	33.96295364038724	-22.47794597320370	10.63760118101682
H	32.47509755622690	-22.94877258000004	9.80962210082238
H	33.59632661464374	-21.82541218687436	9.03648519845391
H	37.06713547548202	-24.28803567882628	10.72824932981171
H	35.92182936744813	-25.42364519107859	11.44419408167249
H	39.84227048644167	-29.19925399364258	8.79428570081043
H	39.45521542283209	-27.55196011888360	9.30283047572172
H	38.42394330504513	-28.89643810412509	9.80240187888916
H	38.76791012681510	-30.95126977676550	5.86674833721054
H	39.80058467016738	-29.69605555682252	5.17424031678287
H	40.01839505734081	-30.19177909348228	6.85634931725299
H	35.57149450557718	-23.69270775695999	11.45782107280504
H	39.62608296106794	-22.86863844658393	3.72441924756003
H	38.65319494395180	-21.60040155496989	4.49151035531381
H	39.45554055341760	-22.82547388055200	5.48383685013743
H	31.74383827769256	-32.02994608774576	5.72139369953341
H	32.95861267903341	-33.32064099313469	5.76434076822429
H	32.91425184007881	-32.10680801154682	7.05333909934701
H	34.77656301557889	-31.58084241666807	5.48710752587585
H	33.63990862874035	-31.55146379555680	4.11765897789272
H	32.25302108915706	-26.66120592227687	7.58931977229361
H	31.86562454701264	-28.38205593114486	7.67856210839636
H	33.17419415441245	-27.72170960118485	8.65993888088504
H	36.91192842292404	-23.00732789723775	2.57706211767869
H	37.59993146555826	-24.77482457160906	6.32687818132452
H	35.05243396964052	-24.70736884104354	3.00503082669589
H	32.20276563484402	-26.83216557994920	2.06954186476918
H	37.20488228398193	-26.56403199230352	9.55986650176709
H	37.61071250091272	-29.60385567322187	3.98089510450906
H	32.33116232511189	-23.15600015045194	7.27430186956958

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B3LYP Scan/Melmid IPC Model/Triplet/300 degrees Constrained Optimization

C	38.93803068615896	-22.74106010510479	4.57651106434795
C	37.73393530428502	-23.62056153228513	4.49299338011486
C	37.17557997627022	-24.50954239045392	5.37558952613677
N	36.91025979150736	-23.67571365527505	3.37577847234506
C	35.91733032229495	-24.57062940641281	3.62189548250299
N	36.05337735572148	-25.08967442544041	4.82308375084984
C	30.37503062693715	-24.71838298793268	2.64472533840658
C	35.92216321385721	-24.67153913362575	10.88708361668313
C	39.18503460774764	-30.02262576832463	5.94429219598362
C	33.41547444314856	-28.65594035205881	0.62578597945627
N	33.17759772498710	-25.50235263261639	5.02113194210239
N	34.77174930454734	-25.49380963048679	7.40723838768240
N	34.78885412310520	-27.56538387663122	3.94926280739687
C	32.75778450526450	-26.67603809208282	2.91392197941580
C	32.96145648626629	-23.92681388299599	6.88733864077322
C	36.57128583065558	-26.64696106294087	8.59696760045648
C	36.83350811606846	-28.86294637517784	4.30853214693588
C	30.57541897818002	-22.80650683091669	5.27318229119190
C	33.55034921510945	-22.78127118629297	9.69980512544682
C	38.92981565373827	-28.62540175904666	8.87507406475957
C	36.22685197960104	-30.03014466974341	1.50680112371663

C	32.4563471449770	-25.71647350251681	3.87491678583454
C	33.95825756465833	-24.43617694297027	7.71275165350987
C	36.96290546197125	-27.50072249429178	7.57310632361856
C	35.73371756385915	-28.47060032073989	3.55343229831837
C	31.36630352762198	-24.76284975163087	3.77021839162437
C	34.24997455843322	-23.93715314489559	9.04796427937616
C	38.08974281170350	-28.41215403317132	7.65099709442829
C	35.40471365315020	-29.01490052770355	2.24471289783173
C	31.45168806366527	-23.95736819419544	4.87605025605931
C	35.24649440086328	-24.73181688906915	9.54908896860398
C	38.19303742863910	-29.00310932406274	6.41950383874706
C	34.22176909522558	-28.43536831152569	1.87141980437629
C	32.58124477227572	-24.44192298878530	5.65173262788749
C	35.56405426656899	-25.69314950922661	8.50685736498332
C	37.10990031608027	-28.46565499506467	5.61224411565050
C	33.85868295717707	-27.52429932805723	2.94433055722847
N	36.38311298277726	-27.55446689280108	6.33113633640670
Fe	34.74375690099061	-26.57563457083130	5.70737040737014
C	34.51508003884891	-31.39086049123675	5.79433870521000
C	33.39881339253577	-32.36181779394749	6.14965457504639
C	32.33791221201185	-27.52450628070832	7.35772577728104
C	33.55692238457605	-27.89905911139251	6.55963538342104
C	34.00138498853479	-29.28112030540075	6.79332556150683
O	34.34318078208874	-29.73086416952489	7.87210721378317
O	34.01960344546520	-30.04589557183126	5.65978279252540
H	29.80783712822142	-22.60698797139380	4.51919424959577
H	31.15316036510378	-21.88212631421179	5.40573435434260
H	30.05769994745577	-22.99954351333032	6.22219875845833
H	30.86490000437393	-24.56526346694023	1.67360930332040
H	29.80431546659603	-25.65365886948024	2.57077593687801
H	29.65336790856383	-23.90643865277227	2.77698046058109
H	33.19765868710620	-27.71264158341116	0.10771794462159
H	33.94295813907564	-29.30233807909841	-0.08254132037336
H	32.44995486840340	-29.13039002014191	0.84678700467018
H	35.81698151498491	-30.23073451638865	0.51189464075748
H	37.26426036227516	-29.69578274013382	1.37339106725521
H	36.26602852651544	-30.98855934860415	2.04195509413332
H	33.96841481305170	-22.56663423951817	10.68814643878198
H	32.47822516040028	-22.97877833697755	9.83317084272102
H	33.63575416011361	-21.86501232844708	9.10047043734148
H	37.00537053924745	-24.51857466252326	10.78942297022622
H	35.78034149887109	-25.60125192429190	11.45379831424873
H	39.76013507989324	-29.31045207357532	8.67839740583283
H	39.36056679186473	-27.68514059235480	9.24441611541266
H	38.33810854570922	-29.05305263063737	9.69524700615065
H	38.70031605031802	-30.97876350831869	5.70567169453050
H	39.70425048861198	-29.68951867562347	5.03597081382563
H	39.94788748678611	-30.22434431456804	6.70261543841354
H	35.52949810571122	-23.85312424092090	11.49836947139074
H	39.68097933693520	-22.98374861590080	3.80490571796612
H	38.68220134676015	-21.67835712768393	4.46941497241564
H	39.41996341527226	-22.86860159253984	5.55009152108505
H	32.58230540829817	-32.29432254101953	5.42551963839867
H	33.77256745636199	-33.39155712201172	6.14985913544201
H	33.00296187605785	-32.14192769509474	7.14297657644218
H	35.30182770886744	-31.40822055671252	6.55032480146179
H	34.94723981086003	-31.62572848513335	4.81895081277941
H	31.93535755079527	-26.55287426177013	7.07697612732238
H	31.53725790509943	-28.26677594445602	7.22634221137199
H	32.55475155313486	-27.49213081395372	8.43697138761702
H	37.02678545232813	-23.14374581538501	2.52513853032749
H	37.50649024050655	-24.77165521701621	6.36947953495846
H	35.13289693916095	-24.81303052618589	2.92028403771839
H	32.09919805024960	-26.74300691652684	2.05394055032649
H	37.11766318158183	-26.70774117585028	9.53222464319659
H	37.50391259197893	-29.59105904129634	3.86331420023527
H	32.39298199182473	-23.08349483937322	7.26575593048416

B3LYP Scan/Melmid IPC Model/Triplet/310 degrees Constrained Optimization

C	38.95042536856374	-22.80185303273729	4.54888586188559
C	37.73281993444401	-23.66384059614022	4.47976980912433
C	37.17127492818928	-24.54389093479491	5.36932547642408
N	36.89705728831254	-23.70905936539771	3.37115942024410
C	35.89472568657823	-24.59018130221707	3.62866407554560
N	36.03588980796832	-25.10965633228055	4.82895165544970
C	30.34023577488461	-24.75103711171418	2.67744335717585
C	35.92632912292045	-24.66083468254054	10.88937661424222
C	39.19624424852083	-29.99901531233070	5.93852150458126
C	33.38771856088599	-28.68684752248226	0.65396412544880
N	33.16243951639409	-25.51800415074190	5.03497296699979
N	34.76540956018461	-25.49956891677761	7.41744241281257
N	34.77018125328933	-27.57806924199777	3.96765649353415
C	32.72127022013179	-26.71398248001755	2.94608265218061
C	32.97502638121989	-23.91574375357433	6.88214055802650
C	36.55094309040683	-26.66565682845467	8.61401554315358
C	36.84041735919794	-28.84063576453146	4.30607900719907
C	30.58737718502522	-22.79532863910757	5.27007160849754
C	33.58554281712422	-22.74556509295770	9.68160794158284
C	38.91659944376272	-28.63956764094144	8.88522054468483
C	36.23501413149165	-30.00491043460213	1.50375222363406
C	32.42860634147814	-25.74382177400727	3.89975564260550
C	33.96742946838481	-24.42754157989071	7.71176316599297
C	36.94281103628227	-27.51869947406871	7.58940996494357
C	35.73000288063979	-28.46203942529271	3.55991477478004
C	31.34332301206745	-24.78502011755108	3.79276738846846
C	34.26709416483709	-23.91887513802725	9.04171862189269
C	38.07656917716888	-28.42237767073569	7.66161727628475
C	35.40010464703479	-29.00800211828639	2.25208864122455
C	31.44836380019050	-23.96133540088099	4.88358173245145
C	35.25034308580170	-24.72462055223523	9.55171981148263
C	38.19124038641584	-28.99660948650252	6.42273127081860
C	34.20112991648772	-28.45329932892146	1.89253374361222
C	32.58156420563270	-24.44316823420780	5.65576072278533
C	35.55410088860208	-25.70041686153876	8.51839684512301
C	37.10635171522482	-28.46029827682953	5.61705296045093
C	33.83086202411585	-27.55076553714685	2.97026374665981
N	36.36613603806201	-27.56756632206968	6.34469189542980
Fe	34.72612080109901	-26.59577828250605	5.72246195213389
C	34.62978387220658	-31.33240437518842	5.83335992566186
C	33.48846355973402	-32.32911587019943	5.96763451291098
C	32.31014815594813	-27.47767832446332	7.38908434882353
C	33.53290367169407	-27.88664851977696	6.61178638619325
C	33.90310725508773	-29.28681767006614	6.82518153684211
O	34.02199436431584	-29.80631842959854	7.92360370665063
O	34.14782589712351	-29.98676877493994	5.67690380311795
H	29.81491660342741	-22.60016589573546	4.51999747252768
H	31.17562846982543	-21.87487755512648	5.38194367492860
H	30.07684152417692	-22.96759778343505	6.22689361900832
H	30.81887643722576	-24.60059655034724	1.70026404590302
H	29.77358478406241	-25.68949360935628	2.61464793264098
H	29.61582378196896	-23.94213784229564	2.81321647758536
H	33.15640646277904	-27.74786737039349	0.13384234939167
H	33.91631123201208	-29.33100681345678	-0.05552670504459
H	32.42880541134581	-29.17013124338972	0.88423458552056
H	35.82662309576857	-30.20180474072339	0.50748362539036
H	37.26753736489461	-29.65519969204852	1.37242687358959
H	36.28767133642610	-30.96779757791177	2.02973650096179
H	34.01546107187677	-22.51975761730158	10.66235733387743
H	32.51280509103413	-22.92983132370051	9.82851416492406
H	33.67447041617557	-21.83994867336186	9.06691474660286
H	37.01349721154397	-24.54085481252394	10.79036847806972
H	35.75722249168896	-25.57586095626442	11.47239291608806
H	39.73710929307313	-29.33691880577327	8.69070580946068
H	39.36140850103064	-27.70286344719277	9.24726385379669
H	38.32217533316457	-29.05381295143788	9.71020385198552

H	38.72080990632176	-30.95179241848783	5.66986110514255
H	39.72656214280163	-29.64114116364883	5.04607577102713
H	39.94937167154229	-30.21426857776816	6.70278914094998
H	35.55709262512163	-23.82079119160841	11.48581253349473
H	39.68127197072469	-23.05676072056877	3.76968779796791
H	38.70918940849727	-21.73566473294100	4.44267503584074
H	39.44109608010727	-22.93497729798239	5.51734530043102
H	32.79629103916751	-32.24264632429020	5.12527423604960
H	33.87647589568842	-33.35341896187942	5.98760058249717
H	32.93687603665183	-32.15366199515463	6.89292734019472
H	35.28888726991510	-31.37776014386517	6.70225102663968
H	35.21479820459442	-31.52086845806991	4.93030285859687
H	31.92324794919879	-26.50721051327223	7.08527042728326
H	31.50230016180594	-28.21329096300344	7.27440109598249
H	32.52360946636588	-27.42350687005424	8.46732736546790
H	37.01245044746702	-23.18020525725179	2.51842661011640
H	37.50864397638787	-24.80909580534692	6.36022055566158
H	35.10036932007223	-24.82320556697986	2.93508582088073
H	32.05514129730372	-26.79121103363672	2.09282671042127
H	37.09637394546859	-26.72770029933245	9.54981936338571
H	37.52364251832524	-29.55027205649253	3.85062808759535
H	32.41781769283748	-23.06112379831800	7.25188509739713

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B3LYP Scan/Melmid IPC Model/Triplet/320 degrees Constrained Optimization

C	38.94577334501491	-22.81876393773685	4.53337904522093
C	37.72468692349888	-23.67629780433326	4.47069025684637
C	37.16937278887755	-24.56075547389067	5.35984934992233
N	36.87756688407888	-23.71135106551737	3.37041388724221
C	35.87527550897209	-24.59142232820880	3.63212824164337
N	36.02704312605963	-25.11967214652435	4.82720435222115
C	30.33371928856780	-24.76263386784943	2.68382789487523
C	35.92253817299962	-24.67348639504737	10.89236384389864
C	39.21433771439007	-29.98005540065866	5.92427231354280
C	33.38323785852932	-28.69695871138951	0.65821311574110
N	33.15530709268165	-25.53209321935073	5.04132985392277
N	34.76680756288292	-25.50650788689126	7.41765155619256
N	34.76339756291444	-27.58849192817235	3.97305617511412
C	32.70924200475290	-26.73213403500982	2.95599458767460
C	32.97780526310763	-23.92122611153763	6.88160474303818
C	36.54842147979433	-26.67681782459232	8.61667374635682
C	36.84689987528535	-28.83249545693964	4.30056259916424
C	30.59395864097317	-22.79554696175641	5.26670498541402
C	33.58930066465046	-22.75085376641776	9.68058195138086
C	38.92607001658473	-28.63931871493839	8.87903180101963
C	36.24316507683806	-29.99397974468548	1.49770472387219
C	32.41924355707295	-25.75939847291935	3.90799623587861
C	33.97019486261998	-24.43310933613613	7.71110676158962
C	36.94316701998073	-27.52600327036577	7.58999593354702
C	35.73042696345415	-28.46199602372560	3.55965310064361
C	31.33736837757241	-24.79676495793548	3.79864817725148
C	34.26887095758660	-23.92574458817079	9.04152756073077
C	38.08325416301514	-28.42253611033329	7.65716901000853
C	35.40142843119484	-29.00681197130077	2.25126630133422
C	31.44774166296153	-23.96859645946937	4.88550118392182
C	35.24864408508324	-24.73484303954835	9.55348898494943
C	38.20150079846891	-28.98870331772903	6.41492682622778
C	34.19646880145888	-28.46173992019504	1.89661406550483
C	32.58009697564042	-24.45199506558971	5.65820108823024
C	35.55259607574715	-25.71026980293806	8.52020203439048
C	37.11156041938814	-28.45644503270022	5.61297374696311
C	33.82176127030156	-27.56509468074333	2.97764973677920
N	36.36480625950281	-27.57423792379602	6.34593714919566
Fe	34.71904943606331	-26.60941197667000	5.72866671388561
C	34.65746359316159	-31.32419453019690	5.88094902109498
C	33.48322552345880	-32.29241228353117	5.87337955396194
C	32.34216549832623	-27.43693694842800	7.45157218708624
C	33.52384089571738	-27.88626625743382	6.63437077358788

C	33.84668275151322	-29.29510043087825	6.83578580937317
O	33.80724012963626	-29.85362628756078	7.92313529765189
O	34.23053596217040	-29.96363354548783	5.70703602441544
H	29.81908869709448	-22.60266031398625	4.51854174679858
H	31.18716460350370	-21.87711965740286	5.36867666448793
H	30.08679315344469	-22.95779535477281	6.22702898498361
H	30.81288321755698	-24.62154453537532	1.70552781375274
H	29.76045812085186	-25.69745982999757	2.62698729443448
H	29.61515619891414	-23.94781068472874	2.81505999556428
H	33.14264347306844	-27.75752697174911	0.14317433358378
H	33.91692942217234	-29.33244710577603	-0.05526854847373
H	32.42914659944009	-29.19028823243628	0.88715158904741
H	35.83249133124692	-30.19369141282692	0.50294156173525
H	37.27149304355564	-29.63361027446382	1.36231591177493
H	36.30769707231629	-30.95674072460655	2.02249572953330
H	34.01487860279620	-22.52935535958959	10.66417798438924
H	32.51497181072528	-22.93054491685985	9.82107500859017
H	33.68585969420247	-21.84418673830554	9.06855696791781
H	37.00890815005467	-24.54452595473838	10.79533508417628
H	35.75980474102189	-25.59317745264366	11.46970472239109
H	39.75245315428219	-29.32844298023864	8.68014345298137
H	39.36280613993991	-27.70083078128937	9.24613407028833
H	38.33604194402465	-29.06310566690439	9.70241177121016
H	38.74694805000159	-30.93602647192854	5.65285243822514
H	39.73897173220995	-29.61354176820588	5.03201014285132
H	39.97132315199585	-30.19157268910002	6.68577413046675
H	35.54613273626293	-23.83982209431803	11.49319281567146
H	39.66783705934224	-23.07062452005952	3.74503864558511
H	38.70714912957138	-21.75105320004796	4.43712387012887
H	39.44584995452828	-22.96039027096678	5.49581657176997
H	32.88922557678536	-32.17306392307713	4.96294030460276
H	33.84104671745580	-33.32694116818761	5.91648559151154
H	32.84037942950076	-32.11537686832156	6.73697188323516
H	35.22237226011057	-31.40843547697981	6.81140704457078
H	35.32682823364694	-31.51012178482579	5.03785227034498
H	31.87346541832806	-26.54120021874355	7.04601983892629
H	31.58158706385117	-28.22406939559101	7.51648273417155
H	32.63465243268865	-27.20987116637944	8.48748981315694
H	36.98611671557299	-23.17717200338400	2.52009868208816
H	37.51616291697383	-24.83397721208480	6.34530446507215
H	35.07369972745528	-24.81786654634668	2.94469489307754
H	32.04140733792319	-26.81102454089844	2.10423062047485
H	37.09302650104225	-26.73977023705622	9.55290864860116
H	37.53613089842727	-29.53291485370838	3.83986182862526
H	32.42357344856110	-23.06389971886614	7.24954202516742

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B3LYP Scan/Melmid IPC Model/Triplet/330 degrees Constrained Optimization

C	38.94062327039136	-22.84597358842942	4.52953179844401
C	37.72170391619749	-23.70704897556971	4.47304576184557
C	37.16556086347047	-24.58268929277823	5.37053281306865
N	36.87755791623283	-23.75605356600336	3.37109014604445
C	35.87609964861885	-24.63496357509346	3.64043282706083
C	36.02553274365049	-25.14950633573196	4.84168202796957
N	30.31304189917056	-24.75752908491069	2.74566913831101
C	35.94389207471411	-24.70842518937759	10.91772718468122
C	39.25278311704763	-29.93223048086453	5.88016824277660
C	33.31290703636427	-28.73419083424963	0.70862569277400
N	33.15988381337050	-25.53401171406263	5.06924352521015
N	34.77651161973078	-25.52664172863964	7.44317117616653
N	34.73214915232283	-27.61421851502755	4.00257465375338
C	32.66862812405908	-26.75675045473791	3.00688345074300
C	33.02142301093597	-23.90715095858805	6.89968490507618
C	36.54682979565695	-26.71637006225737	8.63573818097687
C	36.84008416473968	-28.82417208863059	4.29478966587928
C	30.63721100856316	-22.76433245075355	5.30124062921990
C	33.65731019658099	-22.73789595288220	9.69642413294341
C	38.95181097623674	-28.65033839166609	8.85844714638437

C	36.20022502091669	-30.00130399858460	1.50335656720362
C	32.40451806223207	-25.76656083195597	3.94957675344280
C	34.00460970957020	-24.43388349334052	7.73143654448508
C	36.94100858545924	-27.55291191971532	7.59776598250691
C	35.70359184426010	-28.47551041767937	3.57386504735147
C	31.33308704129836	-24.79204249223658	3.84558521875168
C	34.31304830768309	-23.92833560224840	9.06121544264561
C	38.09579034272632	-28.43232561516066	7.64582076606056
C	35.35898994076921	-29.02434804865279	2.27078799080709
C	31.47108441679182	-23.95201128425548	4.92091344248993
C	35.27324644344026	-24.75763295905760	9.57687192417210
C	38.21926375030851	-28.97364139644450	6.39287254095795
C	34.14246869168333	-28.49230635682076	1.93489297039954
C	32.60657556247518	-24.44154147429900	5.68335604687133
C	35.55888764339875	-25.74126002134143	8.54521464270693
C	37.11415210108538	-28.45036839984103	5.60591261548789
C	33.77734547380948	-27.59553989736929	3.01928398280262
N	36.35815359967880	-27.59162902378868	6.35613380303949
Fe	34.70586844636813	-26.63564172391481	5.75412728670578
C	34.78260464181906	-31.29586465632739	6.16769498592134
C	33.69938275420864	-32.22289937423038	5.63370420787553
C	32.15846066378495	-27.37965526907236	7.20410379115037
C	33.46291538925824	-27.87748556405528	6.64530623857025
C	33.68487873352812	-29.29884518904204	6.87135926403008
O	33.24692170767751	-29.92182603718994	7.83296204840577
O	34.46565016067120	-29.91627363455300	5.93391112666847
H	29.85689514530180	-22.56741796832147	4.55992980972167
H	31.24370707677987	-21.85318386833942	5.38869082198289
H	30.13869970384748	-22.91188015649446	6.26840891767168
H	30.77782991404601	-24.61802543357037	1.76017867639903
H	29.73747439672436	-25.69135357556832	2.69832578211234
H	29.59775702161342	-23.94155704476545	2.88704564319055
H	33.08181527319421	-27.79922699963958	0.18095691788662
H	33.82901985483547	-29.38951496522596	0.00028739173331
H	32.35355926538656	-29.20826407235538	0.95514122636163
H	35.77055765776521	-30.21355577140987	0.51926900039234
H	37.21859514076621	-29.62339842710982	1.34241282865873
H	36.29377491044975	-30.95921843129105	2.03215125766384
H	34.09692286063871	-22.51354651266265	10.67320433298036
H	32.58215920496733	-22.90095932546945	9.85069636800988
H	33.75980355073276	-21.83846765070160	9.07489105058859
H	37.03539116263207	-24.63223634956464	10.82391188130685
H	35.73530092317345	-25.61061132945542	11.50809109158246
H	39.77782861548500	-29.33687196641334	8.64922718149936
H	39.39021605362004	-27.71176165438128	9.22351099502386
H	38.37233503625637	-29.07745078153940	9.68759374438208
H	38.80728276144497	-30.89257166643903	5.58799253774741
H	39.76830793697486	-29.53465417915815	4.99591455856815
H	40.01506902101701	-30.14347058092261	6.63642003188685
H	35.60525329503711	-23.84897411985570	11.50467123384052
H	39.66427151179003	-23.10307850422511	3.74434476770795
H	38.69957279690685	-21.77972214240138	4.42345025861259
H	39.43986507618850	-22.97774443251618	5.49380405699104
H	33.50363056454034	-32.01794119507863	4.57738566520952
H	34.00887018700428	-33.26943692976203	5.72894345056716
H	32.77285597480252	-32.08732027183709	6.19394686980272
H	34.93648641448341	-31.45519001729483	7.23649726554375
H	35.72781505777220	-31.45262742150623	5.64216229321384
H	31.44025251713812	-27.18254260729842	6.39648600634315
H	31.72048200849012	-28.12355938722780	7.87365197641532
H	32.26378046917221	-26.44216007350527	7.75466940159355
H	36.98726294017201	-23.23119262589951	2.51514539271020
H	37.51066715794352	-24.84395242104681	6.35986515282804
H	35.07599425260933	-24.86938592451839	2.95399159968075
H	31.98784620045687	-26.83913483995873	2.16569866921183
H	37.09477395310786	-26.78716307172047	9.56949553966695
H	37.53639348393087	-29.50851575838504	3.82052911135339
H	32.48416725284274	-23.03735771673229	7.26353861051790

B3LYP Scan/Melmid IPC Model/Triplet/340 degrees Constrained Optimization

C	38.93093961439502	-22.85121477419168	4.50910138782683
C	37.70439915599200	-23.70198454143211	4.46238888867094
C	37.16113417045747	-24.59081557781670	5.35473207078680
N	36.83692088426572	-23.72434711449096	3.37782920100249
C	35.83536684946711	-24.60185216215018	3.65144579316674
N	36.00648782291714	-25.14020992277898	4.83926158105521
C	30.30585842383448	-24.79768711326694	2.72158949172025
C	35.93739271253393	-24.65869292892801	10.89555864288493
C	39.24518757296151	-29.93838520881401	5.91739319304519
C	33.34824664593442	-28.74628503993440	0.70380067665029
N	33.14070800397325	-25.55736522064643	5.06604248370826
N	34.76639536214207	-25.51733061250698	7.43247375083562
N	34.74283650609336	-27.61446729539991	4.00434379835175
C	32.67007646396407	-26.78376661586934	3.00298917754826
C	33.00289245297188	-23.90959094606803	6.87643915903049
C	36.53839107236544	-26.69365636451309	8.63877254631276
C	36.85489101029061	-28.81575067409428	4.30824708625015
C	30.62259563938370	-22.77885155797520	5.25850713074573
C	33.64019725917612	-22.71005351466295	9.65754854046308
C	38.93393506217046	-28.63840691411628	8.88785673966830
C	36.24335091828805	-29.98622143491391	1.50996688155188
C	32.39177984427813	-25.79676185739448	3.94413992895569
C	33.98919410170122	-24.42551344664968	7.71103545139356
C	36.93576321559874	-27.53889465901531	7.60950528157566
C	35.72346532510382	-28.46728266789815	3.57932112453688
C	31.32021140349455	-24.82292590046831	3.82686685508552
C	34.29746137659302	-23.90602358170228	9.03427247605365
C	38.08748195320427	-28.42188327342037	7.66834991206448
C	35.38997341053757	-29.01772431583137	2.27459185631728
C	31.45395893441944	-23.97334643157229	4.89436889778974
C	35.26167582932266	-24.72684929770623	9.55785331621994
C	38.21563636368908	-28.97002661987296	6.41911802062387
C	34.16921835610902	-28.49788956434218	1.93458713876760
C	32.58687032362700	-24.45714319028068	5.66636542939333
C	35.55000415652018	-25.71945575667482	8.53669815545650
C	37.11714687577120	-28.44575626522542	5.62288821764102
C	33.79019225422833	-27.60707090153426	3.01868601531934
N	36.35792966526941	-27.58366820832705	6.36545486934016
Fe	34.70273189396821	-26.63773553144659	5.75642431649950
C	34.70888180693068	-31.32374604403070	5.98338735119697
C	33.55737509343074	-32.21422867229008	5.53652149996462
C	32.36701423164013	-27.39492240663979	7.52527911952360
C	33.49917367519543	-27.89815779977149	6.67182800125946
C	33.71221590659653	-29.32996945006565	6.82699797590387
O	33.31406902074009	-29.97845761659365	7.78899916942468
O	34.40974472005179	-29.93106998910863	5.81586747084697
H	29.84601611153466	-22.58703772373086	4.51187422663419
H	31.23213941581879	-21.86901180543675	5.33869830149390
H	30.11941646630556	-22.91382027775214	6.22510857757370
H	30.77655850423004	-24.67940990154888	1.73617735879761
H	29.72209233767875	-25.72705961378368	2.68740408602363
H	29.59747021120169	-23.97283570134799	2.84532899927598
H	33.09466131725655	-27.81107233344796	0.18723915159764
H	33.88254313965322	-29.37926996824019	-0.01138860972791
H	32.40078294203077	-29.24781872727486	0.94194986736142
H	35.82391060994870	-30.19562995323135	0.52087819381156
H	37.26126604987914	-29.60256896991502	1.36068155620442
H	36.33653399485927	-30.94662343051014	2.03449485397456
H	34.07079738121227	-22.48291927350277	10.63765916723553
H	32.56290021677921	-22.86792526891272	9.80132422800013
H	33.75288990775095	-21.81385593339288	9.03300847541035
H	37.02560065047189	-24.54833816555443	10.79625216876338
H	35.76042261517723	-25.56773407555365	11.48547264980863
H	39.76178321003505	-29.32486035175226	8.68583289308085
H	39.36895044055051	-27.69931765900114	9.25563676581673

H	38.34783653577070	-29.06512040169520	9.71259524056440
H	38.79432432179809	-30.89828672349730	5.63213629071368
H	39.76534891317990	-29.55126595928253	5.03124081817103
H	40.00416513407603	-30.14781221263878	6.67750137280726
H	35.57492725270450	-23.81117194788737	11.48547682945374
H	39.63712332413463	-23.10076436487489	3.70575777387692
H	38.69639934432033	-21.78154737641306	4.42543796515957
H	39.44790090241670	-23.00298269996689	5.46103128292525
H	33.26812059710143	-31.98303300398170	4.50741610154025
H	33.85053521783846	-33.26886902900673	5.58170752454565
H	32.69158283959364	-32.07090759751613	6.18450463584780
H	34.96245052915902	-31.51617203658881	7.02797794504948
H	35.59436521086899	-31.48729587959657	5.36425493076347
H	31.93598296521764	-26.47014965489050	7.14568373835750
H	31.57540041648434	-28.14599917982359	7.61181473275840
H	32.70750658849862	-27.19550904329006	8.55180485934266
H	36.93266756929846	-23.18435376634978	2.52964362108043
H	37.52468067844286	-24.87339033074302	6.33149396156001
H	35.02051043651736	-24.81934579854389	2.97685996230627
H	31.99390862288153	-26.87375339162505	2.15893809215728
H	37.08376708737059	-26.75535279725723	9.57470486688786
H	37.55571083441276	-29.49829828100957	3.83809119258618
H	32.46549279893895	-23.03640650019897	7.23186097797866

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B3LYP Scan/Melmid IPC Model/Triplet/350 degrees Constrained Optimization

C	38.93225020760850	-22.87156055669277	4.47373990677271
C	37.70181202131872	-23.71758709176986	4.44887211613939
C	37.17222290928710	-24.60636907684585	5.34953801617207
N	36.81370390205944	-23.73429237913803	3.38104470797782
C	35.8142424589069637	-24.60859974628960	3.67196966041601
N	36.00591068757129	-25.15019606002702	4.85509099530134
C	30.26891769815680	-24.87237175509235	2.78047079085797
C	35.97658153697834	-24.60778820303150	10.89435152229911
C	39.27455389248322	-29.91626290713291	5.94833925451896
C	33.33626098211904	-28.80686684044144	0.76519525908253
N	33.14263604281579	-25.57629458582186	5.09410924173992
N	34.78015165176443	-25.51192712992676	7.45193680208684
N	34.74771228709768	-27.63329562996696	4.04337271570673
C	32.65561071482567	-26.83466407916938	3.05531709882505
C	33.02069024096172	-23.90373908027528	6.88212224748151
C	36.55487689245548	-26.67836038659704	8.66388493094126
C	36.87299371679028	-28.81308173650527	4.34135069029700
C	30.61326981460553	-22.80785236023681	5.27746129962042
C	33.68432499353413	-22.66404889807941	9.64019291504795
C	38.95933433140195	-28.61290274206067	8.91685390084538
C	36.25715562882361	-30.00125814861803	1.55123112847437
C	32.38029073511300	-25.83718336728888	3.98640398091660
C	34.01107418410051	-24.41089328040689	7.71776293446848
C	36.95015114041138	-27.53075547701575	7.63971051584096
C	35.73509827593745	-28.47743463067505	3.61619735602924
C	31.30101145665472	-24.87151085376192	3.86942787529996
C	34.33001859884042	-23.87370352134703	9.03121900727123
C	38.10779247460592	-28.40684248568321	7.69902995959484
C	35.39695504699522	-29.04055767348836	2.31845158787414
C	31.44611580488410	-24.00336182183811	4.92029188108193
C	35.29174778089576	-24.69309536617927	9.56220089644305
C	38.23803077626442	-28.95568795818719	6.45070994536783
C	34.16524286498888	-28.53990815164721	1.98684711733665
C	32.59223695892960	-24.46938769749225	5.68444546958048
C	35.56882779775027	-25.70224651228282	8.55451996829048
C	37.13434427221869	-28.44017214080813	5.65515810332161
C	33.78530521115297	-27.64520945526721	3.06706584666809
N	36.37047401063240	-27.58238333297687	6.39731190456420
Fe	34.70967796047762	-26.64891404679148	5.78796727649782
C	34.63628680212841	-31.33419524188772	5.94840101914517
C	33.55921471683834	-32.08189975035783	5.17420897645759
C	32.38021656774188	-27.37572114576614	7.56518542860220

C	33.49336140046922	-27.89879838317154	6.69923806492620
C	33.60963095085504	-29.34768039439607	6.77108126210969
O	33.00833053841929	-30.04432473678996	7.58390116046254
O	34.46519970523547	-29.91349161701024	5.86580540974365
H	29.82462690255330	-22.63256957501441	4.53946823878651
H	31.21865126500298	-21.89344127153885	5.33384614280990
H	30.12535229307183	-22.93003512355464	6.25351975905947
H	30.72226575294804	-24.76491909987499	1.78572289200896
H	29.69397541392551	-25.80775654087149	2.77036401178160
H	29.55449381169291	-24.05259869103860	2.90327769311085
H	33.07639567704409	-27.87919685343364	0.23821705617168
H	33.86716404422422	-29.44800144070690	0.05479442023389
H	32.39201828463515	-29.30767683262508	1.01693555567960
H	35.83011985928409	-30.22437935369894	0.56842088346030
H	37.26703481652620	-29.60244713751138	1.38799270869837
H	36.37152029356277	-30.95605681523468	2.08160338546330
H	34.12323889548757	-22.42439811790027	10.61362815866748
H	32.60715244218135	-22.81304024269084	9.79402374861041
H	33.79800541674811	-21.77844674591438	9.00095904830823
H	37.06466557106818	-24.50462813013681	10.78628354470019
H	35.79899055850387	-25.50643425435656	11.49985930715454
H	39.78760859628794	-29.29938545699462	8.71662296975882
H	39.39434028342868	-27.67037053454138	9.27592237840853
H	38.37764062172452	-29.03439397955764	9.74738619381691
H	38.83000520203201	-30.87766101084705	5.65829074838265
H	39.79493518434415	-29.52305774049832	5.06493953743462
H	40.03277064516888	-30.12416633425693	6.70964125692075
H	35.62243432220504	-23.74928888926609	11.47334245296811
H	39.62160878575598	-23.12182543047856	3.65611864197249
H	38.70022595414905	-21.80081258100783	4.39725283376930
H	39.46712736789173	-23.02776932230300	5.41497522966611
H	33.52000010760288	-31.73528243811396	4.13757803852376
H	33.76741980246457	-33.15746438954069	5.17025277139992
H	32.58217829524331	-31.92379456630731	5.63343548767883
H	34.63867302164910	-31.63773840805559	6.99705461692681
H	35.62541176849469	-31.51641520376415	5.52065264285811
H	31.99410386721003	-26.41779580947635	7.22336091005500
H	31.55819139786206	-28.09479043873215	7.62194330237406
H	32.72803521419526	-27.23058852170903	8.59877486667806
H	36.89541471127573	-23.19304081130126	2.53220181110938
H	37.55284334251677	-24.89229776503304	6.31880392176672
H	34.98594317457071	-24.82150170926515	3.01250442659004
H	31.97029324470258	-26.94251874439835	2.22082553118192
H	37.10404110569866	-26.73086234465242	9.59823139716417
H	37.57812391419773	-29.49054242387371	3.87026680444641
H	32.48792367997126	-23.02426657668712	7.22898022494411

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B3LYP Scan/Melmid IPC Model/BSS/0 degrees Constrained Optimization

C	38.95905083607438	-22.84839298681932	4.91249706284130
C	37.78261804476151	-23.75239734151370	4.73866442375329
C	37.12030366406087	-24.58221869302477	5.60775040819017
N	37.11017014366148	-23.90423960822125	3.53399685395390
C	36.09808119705225	-24.79567581940375	3.72189169027938
N	36.08141514020487	-25.22129444202871	4.96535520700783
C	30.53972241495760	-24.86531613687788	2.42436741783472
C	35.57495788364599	-24.58300162552201	10.96649928007364
C	39.26840348071644	-29.88531125390784	6.32454228823902
C	33.71237118320670	-28.82431137775332	0.69363636671532
N	33.17726651956131	-25.58645086899980	5.00069535135288
N	34.61605508157940	-25.50971897176364	7.45600959456729
N	34.84867658593722	-27.69652033806778	4.09177878374918
C	32.85724872885992	-26.86225407868229	2.93623885856449
C	32.93854176802824	-23.87718190593788	6.73732140004056
C	36.29035571821377	-26.68125872327272	8.80300108363267
C	36.95075791714228	-28.86365900857285	4.54562748687646
C	30.68901315013633	-22.77459635595462	4.91680264274137
C	33.42124809921396	-22.61100836406095	9.52569799192755

C	38.72361445339347	-28.54867866103741	9.24337359544337
C	36.56401248157657	-30.03165641487861	1.70180785237386
C	32.51449822937075	-25.85246529340145	3.83166074817183
C	33.85383412258876	-24.38845867150551	7.65295240177992
C	36.76610679379701	-27.54579617532296	7.82102971478602
C	35.86828649630938	-28.53690632203516	3.73617400872542
C	31.46639023788766	-24.86915341947743	3.60447376152041
C	34.08478997093813	-23.84155361751005	8.98100967925411
C	37.94161601836055	-28.39149207745445	7.97281983376256
C	35.63736503993545	-29.08635285549061	2.40929547827185
C	31.53035864598935	-23.98796884496098	4.65153897474237
C	34.98878117388932	-24.67235215821322	9.58858304725477
C	38.16980270969631	-28.95477605805842	6.74606270871835
C	34.43853740695422	-28.57672132454622	1.98306865320164
C	32.59715099214735	-24.45967134380310	5.52029482759181
C	35.32054282323452	-25.70052455486630	8.61428446439021
C	37.10970364489815	-28.47708258023407	5.87130878090032
C	33.97295225483505	-27.68981323046841	3.03921407245869
N	36.27444216627629	-27.63018857309720	6.54716119751285
Fe	34.65014917566163	-26.69183056203616	5.82361240395422
C	34.54389620335240	-31.37100659341778	5.97582492416803
C	33.74635474272031	-31.95994591871164	4.82089571859597
C	32.13859305198523	-27.38247650054993	7.23601257463900
C	33.38985057799616	-27.88318693064407	6.57176785837949
C	33.40364629108988	-29.37163435734363	6.56829195987870
O	32.51038624073236	-30.05469065500959	7.04518940318655
O	34.48934532792813	-29.93386890363313	5.98907241577222
H	29.96514073450147	-22.60270478145551	4.11402954162667
H	31.30060259748411	-21.86692169448737	5.00672172273759
H	30.12167514968113	-22.87188835378153	5.85214958487769
H	31.08694942334258	-24.78389689771869	1.47542588244791
H	29.94589959457448	-25.78763932515939	2.37248252303171
H	29.83723274422613	-24.02734068364990	2.46822976440298
H	33.52174420313698	-27.89097748147090	0.14708865219087
H	34.28495496820675	-29.47959150190384	0.02979771572756
H	32.73745941783750	-29.30032182097164	0.86291287034240
H	36.20610730829722	-30.26416634492121	0.69400814060475
H	37.57405354380254	-29.61206604659957	1.60262844194128
H	36.66492866527452	-30.98338121765110	2.24043883307033
H	33.78525247025257	-22.37141043849444	10.52963585253648
H	32.33169017909642	-22.73213400211267	9.59313159691473
H	33.60773760417248	-21.73495756947666	8.89022836418678
H	36.66822114812689	-24.48069698951030	10.93773995314766
H	35.35337829893174	-25.47992751581313	11.55997164905797
H	39.56763387923001	-29.23277603505696	9.11214583499018
H	39.12956406208321	-27.59022164960782	9.59450478882447
H	38.10082665839064	-28.94893110033366	10.05456511514551
H	38.87635416924428	-30.85374404553108	5.98597637125546
H	39.85360727828586	-29.46872335041137	5.49363569737584
H	39.96409307283152	-30.08567718254296	7.14547338723070
H	35.18014494808657	-23.72268261197295	11.51555490550935
H	39.79458237291690	-23.12502217406134	4.25545485468150
H	38.70904620443133	-21.79862414071378	4.70721821164377
H	39.31761956808145	-22.90644372525065	5.94427780432205
H	34.07363291055106	-31.53341507111355	3.86933413240169
H	33.88680863374437	-33.04536537904049	4.78044696039767
H	32.68183863960220	-31.75772220090271	4.94720268823712
H	34.18309231186367	-31.75207652466139	6.93304651689924
H	35.60760409237540	-31.59630591864023	5.87747043751174
H	32.17287665167592	-26.32381271468536	7.47140327542299
H	31.27842158178007	-27.54912386949536	6.57062428302099
H	31.91654338658078	-27.95115598546847	8.14457074962377
H	37.33097165848292	-23.43592181060813	2.66690519653524
H	37.32346616336672	-24.76052671554269	6.65338921739725
H	35.41293986647175	-25.10117808532412	2.94471137506246
H	32.24843301340892	-26.95979601686567	2.04308426993306
H	36.77529265025672	-26.71868605884634	9.77326741301304
H	37.69770549787335	-29.53349084680549	4.13113441884417

H 32.39742483187970 -22.98182971624687 7.02608946409956

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B3LYP Scan/Melmid IPC Model/BSS/10 degrees Constrained Optimization

C	38.97268608306315	-22.87972941036690	4.89764503183586
C	37.78841797016016	-23.77448887805789	4.72941564556963
C	37.11583125591009	-24.58925701036260	5.60480378285557
N	37.11881352931290	-23.93311705607536	3.52402085227672
C	36.09848595906282	-24.81391414663346	3.71769252486401
N	36.07394857896580	-25.22634010491214	4.96541216110956
C	30.53399512888221	-24.85875286644811	2.43246488805196
C	35.57694933244002	-24.57743617687563	10.97116520198350
C	39.24828309447589	-29.90025502394601	6.33380945231070
C	33.70388014274890	-28.81513130490341	0.69640923214185
N	33.16884532791941	-25.58514297486983	5.01006459898206
N	34.61029458387207	-25.50785709785376	7.46367064993680
N	34.83339487398653	-27.70380399637555	4.10237045034760
C	32.84691579522217	-26.85997258251630	2.94477294057583
C	32.93325727304379	-23.87475856316252	6.74624050593102
C	36.28430676360961	-26.68067506951206	8.80934351813452
C	36.93705706476433	-28.86873194536403	4.55366122721639
C	30.68573378473598	-22.76900071479547	4.92538836387280
C	33.42446274895013	-22.60349527366628	9.53091447357884
C	38.70744858772814	-28.56075027234418	9.25206731355096
C	36.55428446271694	-30.02495054813219	1.70218894025089
C	32.50569729292979	-25.85024689155749	3.84080698619533
C	33.85001447472256	-24.38524515466708	7.66054388912622
C	36.75796650938794	-27.54594690979396	7.82702308933632
C	35.85402386283380	-28.54216599882250	3.74455194328254
C	31.45932842459246	-24.86525529226729	3.61359982171052
C	34.08433648276270	-23.83655205007264	8.98743399329671
C	37.92897017455567	-28.39764861616935	7.98013681368367
C	35.62580686010938	-29.08465358732579	2.41413124619721
C	31.52411255966701	-23.98465481990458	4.66113610093477
C	34.98788341485948	-24.66799242152663	9.59457007341139
C	38.15572700354630	-28.96186759733796	6.75359188571920
C	34.42786338235955	-28.57274539157919	1.98798624838459
C	32.58982313911491	-24.45809990848479	5.53010931136695
C	35.31627121771500	-25.69811225724462	8.62090728232148
C	37.09913405686103	-28.47858925049646	5.87778215332061
C	33.96021193872001	-27.69087381847986	3.04729161219792
N	36.26800477919178	-27.62703910997183	6.55254833356095
Fe	34.64001909775106	-26.69234395636444	5.83171180948960
C	34.54091480042882	-31.37382149715528	6.02118188059050
C	33.89251898099805	-31.90111654194275	4.74915666278628
C	32.13930680378865	-27.38896212847085	7.26298419905155
C	33.38008262194744	-27.88240143099205	6.57325198263892
C	33.35782217171860	-29.36839111229991	6.49071583451342
O	32.37782335899300	-30.04238190572998	6.76722886936779
O	34.51783899392355	-29.93669659692116	6.09043498267425
H	29.95901646737153	-22.59886591919145	4.12482789676751
H	31.29916118137448	-21.86197388459505	5.00945448729098
H	30.12193184794049	-22.86191062574521	5.86326747544693
H	31.08230917856983	-24.77368085501544	1.48444441597301
H	29.94126477863868	-25.78151998862264	2.37704129259595
H	29.83063912957143	-24.02161033309864	2.47807765110721
H	33.49930458468599	-27.87818207224867	0.16145007159583
H	34.28480985845070	-29.45436766632309	0.02420620195205
H	32.73613756600648	-29.30718703411114	0.86122014159322
H	36.20376279287017	-30.24240484243116	0.68845591921111
H	37.56683758543058	-29.60847509667863	1.61735881099133
H	36.64662063950505	-30.98465482815702	2.22818915443492
H	33.79064495981922	-22.36277663676456	10.53379156904765
H	32.33472571180328	-22.72195158591122	9.60030781136015
H	33.61190218704374	-21.72911913396032	8.89342979238919
H	36.67032576785792	-24.47722815702734	10.94011464692859
H	35.35493247283476	-25.47297018330341	11.56662164894061
H	39.54866847352925	-29.24840329958601	9.12142520324428

H	39.11694202014295	-27.60489735764343	9.60614992674564
H	38.08102745722633	-28.95986024546359	10.06105577713800
H	38.84947077789050	-30.86606611047383	5.99562844723641
H	39.83730000987449	-29.48873128652306	5.50308907428636
H	39.94169213148406	-30.10502280656889	7.15557980214549
H	35.18471983149522	-23.71551937512776	11.51957719910089
H	39.80681635547103	-23.16999470687799	4.24472190280935
H	38.73297733999834	-21.82951518217768	4.68266260626102
H	39.32884998988615	-22.93210863947224	5.93056536124466
H	34.34641065845732	-31.44445369699050	3.86651095376449
H	34.02262381981174	-32.98678300994780	4.68420564463252
H	32.82404853446999	-31.68323590923373	4.74465795533330
H	34.04847157915350	-31.78233655155548	6.90641311992565
H	35.60325972045900	-31.62257858051826	6.05521691358526
H	32.18544494966557	-26.33638791506689	7.52289986797975
H	31.27063933862469	-27.53713673503387	6.60580159978582
H	31.92335434792896	-27.97444710910659	8.16350264927401
H	37.34706785905175	-23.47641486945147	2.65268599323652
H	37.31412863320861	-24.75877871670718	6.65282883951046
H	35.41407692969304	-25.12243879431611	2.94104273070824
H	32.23879946307120	-26.95447170922098	2.05083885292712
H	36.76908299360036	-26.71953321030709	9.77965180182528
H	37.68237839870159	-29.54050204262341	4.13941421532922
H	32.39344391728108	-22.97847412706900	7.03453951380800

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B3LYP Scan/Melmid IPC Model/BSS/20 degrees Constrained Optimization

C	38.94356757768221	-22.85251194419875	4.90653487408289
C	37.77235681701020	-23.76375115031420	4.73511074963708
C	37.10831868038807	-24.58711957328449	5.60900207082010
N	37.10754678463948	-23.93088146789222	3.52827390086928
C	36.09803977640744	-24.82451458184604	3.71960105264901
N	36.07566071051929	-25.23710315495979	4.96740043193857
C	30.53165534892744	-24.85682411725351	2.44336596793288
C	35.61175243034477	-24.56652945473971	10.96324432062822
C	39.23440206256816	-29.92738131810063	6.33351208712299
C	33.71077679352561	-28.79388451819856	0.68413779395596
N	33.17461709033010	-25.58190202165894	5.01266905257286
N	34.61829991730950	-25.51024655526645	7.46642922726417
N	34.82732974637110	-27.71454562059351	4.10489888561586
C	32.85238932527837	-26.85027861455218	2.94258193196151
C	32.93529803349671	-23.87981956771269	6.75650047405296
C	36.30044168429725	-26.67881503456663	8.80561552993215
C	36.92079341370682	-28.89521048873086	4.55982796515918
C	30.67338763033935	-22.78167098177467	4.94923591766626
C	33.44365823969049	-22.60100227577319	9.53440586037850
C	38.72142785448165	-28.56064499745312	9.24406928862565
C	36.54706891926074	-30.02782317987008	1.69560608251465
C	32.51088717158926	-25.84464110618379	3.84307767915306
C	33.85826634821406	-24.38751600903001	7.66574986087447
C	36.76442007909660	-27.55121405185150	7.82530668686632
C	35.84343793233909	-28.55838276674331	3.74722546967645
C	31.45942280378275	-24.86368688948438	3.62255560098003
C	34.10119833158430	-23.83475917603056	8.98963258298927
C	37.93259812741091	-28.40689309660742	7.97730236894032
C	35.61982144981829	-29.08895798321495	2.4111055528567
C	31.52023525828691	-23.98926599505086	4.67548609587760
C	35.01080565265590	-24.66275109369846	9.59211099645180
C	38.14767243499114	-28.98271120244964	6.75426526494690
C	34.42869650654496	-28.56476060356495	1.98129976771490
C	32.59032531993851	-24.46123422640768	5.53991923680866
C	35.33231252950551	-25.69610325600016	8.61931612554761
C	37.08809810004234	-28.50019443049929	5.88155956781066
C	33.96071027301954	-27.68774252165701	3.04418651165386
N	36.26578441027768	-27.63867100147064	6.55451615364159
Fe	34.64087447604182	-26.69599250871716	5.83506809501130
C	34.45148295152772	-31.40701758081259	6.12118485379200
C	34.03060199443529	-31.90621855109275	4.74691830489562

C	32.12893734324774	-27.37381693050297	7.24699577189231
C	33.36781016631264	-27.87465774006729	6.55733192506252
C	33.29226776398536	-29.35099678434113	6.38456334455398
O	32.24416154643137	-29.97460776543655	6.42498518807383
O	34.48145489356343	-29.96893456571671	6.20397605159258
H	29.94664612648575	-22.60944773994273	4.14914929096278
H	31.28041300159951	-21.87125744184592	5.04233678574198
H	30.10887348574719	-22.88686263559503	5.88540967969403
H	31.07802289187223	-24.76933580839190	1.49445688339197
H	29.94057126206669	-25.78062175821009	2.38777169085904
H	29.82694702091520	-24.02098591243158	2.49169549989229
H	33.50893533104006	-27.85182643470021	0.15726720575750
H	34.29452328443025	-29.42704640648503	0.00862024378164
H	32.74219160343451	-29.28726559675834	0.84000708308679
H	36.20987038429236	-30.22040274978676	0.67237939403673
H	37.56594995621029	-29.62282846578294	1.63500079697959
H	36.61944799774775	-30.99963649403190	2.20245612150465
H	33.81555894558181	-22.35804764009581	10.53464024579489
H	32.35441895699297	-22.72005041494643	9.61038866886690
H	33.62666399336336	-21.72779137549196	8.89405464345883
H	36.70453286113480	-24.46331020277218	10.92203527478814
H	35.39789530841087	-25.46093951847535	11.56336361354508
H	39.56071703035846	-29.25037392191060	9.11188591765377
H	39.13537963523907	-27.60240292378542	9.58639053776453
H	38.10174813571837	-28.95197494482770	10.06199572906996
H	38.82957502302444	-30.89046739781112	5.99505167642200
H	39.82535292888960	-29.51894239039648	5.50253880457858
H	39.92731593176830	-30.13637196316250	7.15466727508155
H	35.22205026161711	-23.70409886334320	11.51266155089117
H	39.78321234226753	-23.12998705569024	4.25513520624040
H	38.68911163718493	-21.80566687566210	4.69191662538399
H	39.29808047658617	-22.90054975814357	5.94021982319385
H	34.66670595001435	-31.48091688421490	3.96766446992618
H	34.11281742172740	-32.99769374214760	4.70468311606402
H	32.99594575257262	-31.63097070770701	4.54197834553103
H	33.78092041832121	-31.79210860139057	6.89288502860310
H	35.47494889258159	-31.70547280024008	6.35548196486452
H	32.24034629809677	-26.36599900096125	7.63550952738172
H	31.29572711444642	-27.36343698434633	6.53035568676891
H	31.81383679902256	-28.04213600772330	8.05537837871385
H	37.33145162868831	-23.47083831331999	2.65757193757532
H	37.30656472783257	-24.75421632644032	6.65739258065547
H	35.41826602358667	-25.14014247727390	2.94175911799170
H	32.24584367645802	-26.93850542569845	2.04695641512287
H	36.79221711887110	-26.71326467359282	9.77256457220749
H	37.66084635943840	-29.57392309757695	4.14750989743544
H	32.39330028814472	-22.98602990451738	7.04841377726141

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B3LYP Scan/Melmid IPC Model/BSS/30 degrees Constrained Optimization

C	38.95093966602913	-22.86490579789222	4.89474925556277
C	37.77119739892482	-23.76500211645037	4.72333005858827
C	37.10189481861031	-24.58521561160749	5.59611855470498
N	37.10283031677849	-23.92314834440843	3.51721907632082
C	36.08605202793920	-24.80861540722512	3.70787087760742
N	36.06272512588780	-25.22464654957211	4.95454879688016
C	30.54234242536118	-24.78100015171134	2.42635189262913
C	35.60090661243181	-24.60406822264020	10.96516648811554
C	39.18756743642515	-29.96539326557469	6.29655161737850
C	33.66701832831335	-28.75764094333457	0.66094167371828
N	33.16495067347272	-25.55451792177056	5.00294356435014
N	34.60817097405069	-25.50986556356981	7.45813444656179
N	34.80495824098793	-27.69536986172751	4.08015832643912
C	32.84116518341490	-26.80156210239750	2.92001677205715
C	32.92325845752294	-23.87348919693449	6.76664120280076
C	36.29390101014425	-26.68997520352117	8.78289323209655
C	36.88542022172267	-28.90004276519307	4.52934103006639
C	30.67883865619527	-22.74002391741393	4.96030628619652

C	33.42450186594470	-22.62994944880270	9.56168681881245
C	38.69625532720841	-28.59839704241636	9.21123571288870
C	36.48353522491063	-30.03758539041909	1.67051200934455
C	32.50570861477499	-25.79970078639434	3.82724712693791
C	33.84467743679302	-24.39211722033298	7.67122997567690
C	36.75392412642259	-27.55655228236980	7.79576337831675
C	35.80856663124537	-28.55314695985250	3.71982256573753
C	31.46182584093794	-24.80922934906549	3.61167125534775
C	34.08631115656057	-23.85450585360919	9.00158983392752
C	37.91119664847227	-28.42761861846710	7.94439485030305
C	35.57429455921080	-29.08073433417531	2.38449906752931
C	31.52035311876516	-23.94905825432268	4.67625600869969
C	34.99999252066352	-24.68581166750936	9.59312950119265
C	38.11769606310602	-29.00290304231639	6.71975273930609
C	34.39149845451522	-28.53756035647860	1.95600067644467
C	32.58294701383601	-24.43774444878462	5.54077276398404
C	35.32425855296891	-25.70650185234087	8.60792150548088
C	37.06440638414490	-28.50293053211193	5.84911839379274
C	33.93763857977204	-27.65425833725535	3.01969290768928
N	36.25533527012948	-27.63168138960713	6.52431787324815
Fe	34.63049325028285	-26.68052698626777	5.81619205242663
C	34.45986615872171	-31.41678271677936	6.34165929187812
C	34.36296270054943	-31.95452536559270	4.92207792209944
C	32.11058558732768	-27.38691188064089	7.19285835347605
C	33.37013068089622	-27.86557693271086	6.52371737728524
C	33.30968564995803	-29.33938902494247	6.31815058004902
O	32.26596913307217	-29.94302412239548	6.14341944034734
O	34.50121672026402	-29.97587986146707	6.39059196831941
H	29.95519543454113	-22.55552855115118	4.16013270395741
H	31.29015475349962	-21.83368189326875	5.06474690514053
H	30.11104455663581	-22.85211442901067	5.89370071316521
H	31.09594795211382	-24.68622420852821	1.48234671829916
H	29.94440522568397	-25.69933901221230	2.35535656835998
H	29.84386236928013	-23.94023806851330	2.48000238951158
H	33.47161236518738	-27.81277311970878	0.13666607456804
H	34.24287231331174	-29.39431279822329	-0.01799366625181
H	32.69457485189804	-29.24257388136616	0.81947766822286
H	36.13671340628006	-30.23395120583822	0.65118836485501
H	37.50770853310278	-29.64775922935205	1.59956648951921
H	36.54543711321684	-31.00617708632236	2.18500420886532
H	33.79503800091825	-22.39865690323112	10.56519197349557
H	32.33556680792186	-22.75323120825384	9.63536776996135
H	33.60511897588319	-21.74792368129308	8.93279135390832
H	36.69364128601936	-24.50019028859860	10.92508419614526
H	35.38733631996093	-25.50493762773342	11.55572617643398
H	39.53174642588117	-29.29182172585005	9.07430898123607
H	39.11496245434211	-27.64608711827370	9.56402166257556
H	38.07229601525071	-28.99404775245749	10.02390595326492
H	38.76582930277886	-30.92438126047663	5.96707785902889
H	39.77806496511079	-29.57089549170294	5.45862860798815
H	39.88354341671215	-30.17971886203376	7.11375268996522
H	35.21096465722702	-23.74765726450760	11.52381183429612
H	39.78745342764396	-23.14985352042036	4.24253121007422
H	38.70631830321803	-21.81551555863999	4.68119230720341
H	39.30577237332835	-22.91723131817695	5.92812273742021
H	35.18658230557232	-31.58189338174714	4.30999225627008
H	34.40725413231386	-33.04890047016740	4.93483599842880
H	33.42189310756599	-31.65367785788212	4.46149541728808
H	33.61826285372255	-31.76603067193237	6.94383139784318
H	35.39254191329258	-31.72279882003427	6.81899300186351
H	32.20826651550829	-26.38608769199773	7.60384680993303
H	31.29715209901686	-27.36649491188121	6.45477773410776
H	31.77895265493307	-28.07073691782864	7.98258014080939
H	37.32928256438831	-23.46293327915361	2.64728362282970
H	37.30049083360200	-24.75709438632915	6.64366038588108
H	35.40245844899586	-25.11690467194979	2.93045245477022
H	32.23611076206007	-26.87707159931733	2.02218530176495
H	36.78591864781626	-26.73415186165577	9.74934922519953

H	37.61547474095035	-29.58854436851699	4.11528733539930
H	32.38102295264614	-22.98310513708846	7.06841706378520

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B3LYP Scan/Melmid IPC Model/BSS/40 degrees Constrained Optimization

C	38.92598895706487	-22.84309844828775	4.90657310562238
C	37.75518039067153	-23.75379997867431	4.72976698158745
C	37.08402957969891	-24.57350254638863	5.60159544206092
N	37.09890030921041	-23.92427315644215	3.51874652315948
C	36.08733265021691	-24.81645782783211	3.70550976104093
N	36.05549175279840	-25.22483789382317	4.95465086320591
C	30.55352148281656	-24.74773321156828	2.41625113126019
C	35.62001163779988	-24.60155411031237	10.95664085786130
C	39.16305289521063	-29.99296004369376	6.28829738360964
C	33.65725355760808	-28.73597719480524	0.64538618587665
N	33.16152491946684	-25.54493442588137	5.00016086889297
N	34.60370418591910	-25.51213970631585	7.45715944345985
N	34.79530138181050	-27.69292122109508	4.07100969665639
C	32.84374081263019	-26.77700108076425	2.90709517971629
C	32.91780114263301	-23.87407169271795	6.77310684600631
C	36.29913706859534	-26.68954516407748	8.77184235685784
C	36.86144441723011	-28.92007494173278	4.52397928279457
C	30.67898768260483	-22.72733675545328	4.96748667834663
C	33.43049867801511	-22.63218391320413	9.56660316953444
C	38.69799704230181	-28.60176498364387	9.19521944255208
C	36.44852603382449	-30.05782358925160	1.66524661404735
C	32.50805284675951	-25.77994464743824	3.81924967340942
C	33.84129913312020	-24.39482667438195	7.67434087888614
C	36.75221777641303	-27.55970849712756	7.78476912100774
C	35.78947855792864	-28.56261984925733	3.71225153238589
C	31.46695048204776	-24.78597824259258	3.60588664914870
C	34.09000353046013	-23.85654547898673	9.00338734406126
C	37.90584159062768	-28.43572419122097	7.93211842405651
C	35.55274700013801	-29.08608108553128	2.37578061383974
C	31.52069636202813	-23.93480661556135	4.67765225705244
C	35.00877230507885	-24.68590769550116	9.58929084312030
C	38.10175544827001	-29.02062681669539	6.71044527608889
C	34.37925400741427	-28.52611220007303	1.94349746152324
C	32.57904478195164	-24.43140527558511	5.54326371932535
C	35.32728516073012	-25.70723550774011	8.60241684042442
C	37.04708902629093	-28.51921814485639	5.84201728245157
C	33.93210516404947	-27.63979168786729	3.00746114799621
N	36.24729095945749	-27.63846992190681	6.51569972215930
Fe	34.62561204607719	-26.67827808651858	5.81033510645369
C	34.36153605067664	-31.44149453898967	6.39780920599526
C	34.55009786222229	-31.96005592203049	4.98094153722434
C	32.12892314855130	-27.41484075936488	7.22636074147636
C	33.37159774447078	-27.85928168103025	6.50543845774430
C	33.29138601181078	-29.32333003920503	6.22833680313434
O	32.26800687581467	-29.87879165193984	5.87596625945269
O	34.43465611117303	-30.00153946028016	6.47800612502636
H	29.95559149869090	-22.53901335960422	4.16796330243952
H	31.29007846554049	-21.82133691271065	5.07660998476414
H	30.11087023353047	-22.84411014077581	5.90010930972368
H	31.11190323981154	-24.64443711503152	1.47592754227271
H	29.95661783807020	-25.66583537269613	2.33430632879913
H	29.85430726331514	-23.90781731513227	2.47366879509817
H	33.45667029368680	-27.78650316833946	0.13169396427287
H	34.23779065361170	-29.36150534582940	-0.03999036239508
H	32.68766454101477	-29.22873202930210	0.79746634451795
H	36.12438245779606	-30.21917887683387	0.63231827783435
H	37.48708338589815	-29.70304592894491	1.63142614724502
H	36.46101352468919	-31.03920695612146	2.15874709085417
H	33.80566955637261	-22.40069466683427	10.56835926452400
H	32.34192259561686	-22.75575110360761	9.64532860544394
H	33.60779560784619	-21.75007588395898	8.93683550921224
H	36.71232797062882	-24.49665481283773	10.90808494487551
H	35.41207277965826	-25.50165647163776	11.55043306376923

H	39.53071466295226	-29.29832254633277	9.05719651281192
H	39.12168270474301	-27.64866513374321	9.53992090550149
H	38.07807702342843	-28.99093566550285	10.01410114797732
H	38.73395700344808	-30.95434068461142	5.97543997774953
H	39.74681146127040	-29.61178484160754	5.43958543082439
H	39.86656565998742	-30.19999578675635	7.10097650045791
H	35.23353756971341	-23.74458595012086	11.51690517409613
H	39.77044116702974	-23.12416382568090	4.26295370715601
H	38.67436057575230	-21.79688435358479	4.68557755370935
H	39.27227301024906	-22.88714322185179	5.94321778230670
H	35.49576679810665	-31.60929187444240	4.56314582814734
H	34.55886234080318	-33.05541632263206	4.98514314322651
H	33.73725461733049	-31.62459699415770	4.33567074303603
H	33.40251338993981	-31.76868436601901	6.80445522218506
H	35.16466855915195	-31.78223018623086	7.05377868883163
H	32.14785037444832	-26.36612302935762	7.50550821457292
H	31.25839996126819	-27.59412316112616	6.58286943884380
H	31.95875123550372	-28.01510295127365	8.13124512967769
H	37.32936246474904	-23.46731469690726	2.64815697186868
H	37.27450324012901	-24.73756725623556	6.65186471880900
H	35.41229999444298	-25.13345805235418	2.92416672247898
H	32.24212091395372	-26.84375613458708	2.00627426570453
H	36.79745465785756	-26.73164633228577	9.73519432168300
H	37.58568511463298	-29.61545238624052	4.11117593346813
H	32.37601401664004	-22.98458832151197	7.07840071403002

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B3LYP Scan/Melmid IPC Model/BSS/50 degrees Constrained Optimization

C	38.93126391273070	-22.83696551631706	4.90658871282354
C	37.75813824158656	-23.74454323040528	4.72936079949412
C	37.08014464957414	-24.55768925088906	5.60196812240539
N	37.10762255860317	-23.9195224515551	3.51584061636107
C	36.09243825667325	-24.80763379836218	3.70204429017319
N	36.05306447755191	-25.20938651563537	4.95314374429968
C	30.55454735739498	-24.71896807788885	2.41336176176242
C	35.63477160908998	-24.59513351178521	10.94993508733642
C	39.13478817689790	-30.01989723917903	6.28330382989159
C	33.63426235978903	-28.72708029389966	0.64333405475442
N	33.15774816661981	-25.53020822502951	4.99795944643776
N	34.59975223065301	-25.50806057467987	7.45600606003315
N	34.79506784678603	-27.67384762035655	4.05769925481240
C	32.84603343469222	-26.74920239849951	2.89646124074981
C	32.90317937811103	-23.87583066565707	6.78447469258615
C	36.30600680385781	-26.68131532546971	8.76038614332223
C	36.84607327365794	-28.92369973377368	4.51538023485864
C	30.66304860146915	-22.72308069939610	4.98411972091029
C	33.42451725880991	-22.63721723912669	9.57726727873597
C	38.69071053649623	-28.61008177882257	9.18420754505786
C	36.41227356767750	-30.07611117251677	1.66444062739049
C	32.50842070972825	-25.75716174753159	3.81324161578871
C	33.83235208384777	-24.39556016691353	7.68023139286907
C	36.75402060976218	-27.55330373684381	7.77276562489918
C	35.77822833742227	-28.55726302905332	3.70200058060289
C	31.46435547052393	-24.76508392359115	3.60547373281082
C	34.08622133553533	-23.85795771276321	9.00863960908329
C	37.89980490888296	-28.43911987693960	7.92097155224362
C	35.53179500652261	-29.08669044945974	2.36953640987098
C	31.51042770881631	-23.92452753871992	4.68580981737053
C	35.01398347892316	-24.68242704134123	9.58701749794329
C	38.08754266574756	-29.03094416170752	6.70149670041478
C	34.36435224405106	-28.51491063481366	1.93647356406942
C	32.56843850679926	-24.42487966181861	5.54983675719363
C	35.33109719350941	-25.70100759680100	8.59661743747671
C	37.03736454095452	-28.52113858934147	5.83231933280448
C	33.92955071322280	-27.61766453697020	2.99612968828782
N	36.24699270592982	-27.63071035564650	6.50420887624577
Fe	34.62691939075459	-26.66487029741194	5.80112871597935
C	34.29365331562843	-31.46036179604986	6.44196620358397

C	34.70255217437546	-31.97003289542310	5.06950950808960
C	32.14563007057155	-27.45392831979902	7.21787274753047
C	33.38777015946781	-27.85778499796567	6.47419842365610
C	33.32180771594395	-29.31010065053234	6.13557377762356
O	32.36058421225154	-29.82470505146011	5.60017823915159
O	34.39237334243711	-30.02235485766295	6.55605218516236
H	29.93853886810878	-22.53276170207051	4.18606450597769
H	31.26972792925408	-21.81481246807164	5.09919717224063
H	30.0956669975988	-22.84865229513691	5.91604758074685
H	31.11560473888395	-24.60803375869147	1.47554129826438
H	29.95886516174864	-25.63707383728233	2.32269776004215
H	29.85426861508014	-23.88022040604937	2.47497331406282
H	33.44194689335446	-27.77968424839014	0.12263812219028
H	34.20440571801052	-29.36475163857730	-0.03952396323172
H	32.65998283724122	-29.20736387581548	0.80467239280161
H	36.07782230023884	-30.24809688581563	0.63653643770918
H	37.45406915421177	-29.73235221185854	1.61712358974634
H	36.41886878938337	-31.05030882711299	2.17173225058587
H	33.80458053409418	-22.40506350162516	10.57703342989182
H	32.33693710097265	-22.76541160100216	9.66227317430614
H	33.59419353646466	-21.75359058498712	8.94750225770175
H	36.72637970217199	-24.48704370050333	10.89346003344414
H	35.43388629195940	-25.49507878216719	11.54643390407206
H	39.52018274051100	-29.31043318646152	9.04594839200041
H	39.11869151042661	-27.65932530265228	9.53001937813553
H	38.06866892259620	-28.99705084762618	10.00257535272510
H	38.69214572173595	-30.97974730624806	5.98451359219072
H	39.71741936417757	-29.65576476290452	5.42647104535758
H	39.84103755013970	-30.22615049265179	7.09381986659958
H	35.24988307048752	-23.73862906968272	11.51205098999774
H	39.77829256447534	-23.12587883942729	4.26985283989762
H	38.68498091359545	-21.79141359238620	4.67671139431292
H	39.27159095143780	-22.87493108883432	5.94543818258287
H	35.71791378781848	-31.65158641109648	4.82591671451447
H	34.67021555356417	-33.06482169848996	5.05651307588393
H	34.02508416956388	-31.59562838361969	4.30136919551970
H	33.27063094776016	-31.76086252693188	6.67674007639494
H	34.96524816909430	-31.83173438290218	7.21814380935324
H	32.14178504160233	-26.40728717183291	7.50719804842309
H	31.27013710333077	-27.65266183733269	6.58684069954121
H	32.01165327745887	-28.06621641990701	8.12170625137413
H	37.34430722483282	-23.46832334032128	2.64393623405840
H	37.26457086569723	-24.71675948716295	6.65408072127037
H	35.42092130685567	-25.12764684070061	2.91896347437140
H	32.24462054659735	-26.81212350323616	1.99521318618192
H	36.80816000948248	-26.72340081715566	9.72178159269804
H	37.56209301089025	-29.62861441280030	4.10452049679241
H	32.35714648959732	-22.99107930607197	7.09600257432188

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B3LYP Scan/Melmid IPC Model/BSS/60 degrees Constrained Optimization

C	38.92150800657788	-22.82244629605773	4.92679103123940
C	37.75054468710709	-23.72930675569728	4.73243273561894
C	37.07498875911144	-24.55981843611073	5.59037519387417
N	37.09918258103069	-23.88273494526011	3.51643547343786
C	36.08564109337284	-24.77594882982256	3.68698577601957
N	36.04827148108397	-25.20097241922790	4.93044698162035
C	30.58145851165758	-24.63565480460987	2.37116089372907
C	35.60199275912208	-24.67659384244624	10.94540070321352
C	39.11776876181149	-30.03564804256985	6.20790832546270
C	33.61384599486105	-28.67138545908217	0.58284221249691
N	33.15662390727206	-25.50733868833253	4.96445135164359
N	34.59284256946106	-25.52083656888720	7.42701872238410
N	34.78306325903396	-27.65127964387866	4.00455097346351
C	32.84988454394317	-26.69355354982635	2.84369572460177
C	32.89558955137676	-23.88135440655283	6.77666938373054
C	36.29759038961367	-26.71288499835571	8.71729861947625
C	36.81420837311842	-28.93613854961855	4.45892622294722

C	30.67590877894026	-22.68724142080001	4.97881944845371
C	33.38939592617475	-22.70206518146387	9.60058435222191
C	38.68367265679189	-28.64439201505984	9.11926057357413
C	36.35915889402772	-30.08052158793516	1.61030026067282
C	32.51545401962293	-25.71063157539183	3.77120688225289
C	33.81990091389309	-24.41652924677181	7.66875849295718
C	36.74576413422297	-27.57379664103657	7.71992358404459
C	35.75102968256260	-28.55141805656117	3.64786311264334
C	31.47950535322223	-24.70802433536355	3.57078412685020
C	34.06308171344424	-23.90534592517693	9.00955345109141
C	37.88912336099395	-28.46422271970028	7.85966337444649
C	35.49743404679530	-29.07358616288103	2.31388638541429
C	31.52041904333349	-23.88701604220131	4.66593493330609
C	34.99200918377287	-24.73656036263698	9.57622529113113
C	38.07031860507129	-29.05121160947196	6.63684191163556
C	34.34343099491696	-28.47736739144915	1.87896203289501
C	32.56920203201563	-24.40765601693679	5.52987153840051
C	35.31983923937643	-25.73326783562564	8.56733558124671
C	37.01784623662387	-28.53413673027794	5.77450452052869
C	33.92137307181164	-27.57719225868338	2.94143070378662
N	36.23592841001173	-27.64089275342346	6.45199914040578
Fe	34.61997197500377	-26.65734620053667	5.75709929720629
C	34.28942148132415	-31.44374899496780	6.70494574160472
C	34.88734737570218	-32.00224056034729	5.42404048047850
C	32.14951897134961	-27.46511947818807	7.18534147638662
C	33.39409893208024	-27.84924365436494	6.43568512545126
C	33.37469403928839	-29.31587147953835	6.15804864080338
O	32.50357730124903	-29.85494056264763	5.50731700648083
O	34.36598549478891	-30.00064092497974	6.77347221619481
H	29.95628470875229	-22.48165681543428	4.18009518386960
H	31.28498598761257	-21.78299516316416	5.11177580065002
H	30.10303785828690	-22.82582378874408	5.90556956062236
H	31.15230040844334	-24.51102945670409	1.44095108069323
H	29.98194965166063	-25.54881812632522	2.25815306941134
H	29.88503581912340	-23.79432637475283	2.44106451950719
H	33.43500514697448	-27.71803448467507	0.06819086749608
H	34.17775006851750	-29.31133992923561	-0.10306397461530
H	32.63313985828177	-29.14041243691153	0.73847755693138
H	36.02258311980579	-30.24682502261104	0.58212617565951
H	37.40766019452075	-29.75750213062030	1.56366628426670
H	36.34615873152067	-31.05404533024083	2.11891804357992
H	33.76109987857695	-22.48968686007226	10.60787563126854
H	32.30217318550760	-22.83971577457280	9.67518777022443
H	33.55693695066326	-21.80333869444171	8.99194355907162
H	36.69366565226211	-24.56404534562445	10.89979034535283
H	35.39956231485736	-25.59013723911696	11.52040900692653
H	39.51302832344035	-29.34342831746653	8.97356958081888
H	39.11211357340112	-27.69620546032556	9.47135607593053
H	38.06381075514836	-29.03798715340381	9.93618432993457
H	38.67847814430149	-30.99573223184364	5.90475757695903
H	39.69518885333854	-29.66407769430041	5.35073462331520
H	39.82836820226827	-30.24465260854079	7.01393077556280
H	35.20994570309969	-23.83381365887867	11.52313201321752
H	39.76869499255235	-23.09583968685709	4.28344703671322
H	38.67204272568534	-21.77305793501199	4.71869834454355
H	39.26280420373265	-22.88075343541519	5.96439332923509
H	35.92308095714355	-31.67768895244419	5.30607099819336
H	34.86843409448725	-33.09700788943736	5.45293038191757
H	34.31691057604283	-31.66948545081905	4.55616607672786
H	33.24469151326241	-31.74434945538795	6.80725967556971
H	34.84680168320551	-31.77841311783190	7.58156921762748
H	32.06871313264308	-26.39746676295129	7.36610731324294
H	31.26892407704818	-27.80083969399456	6.62293103370838
H	32.10942120474937	-27.98429334499005	8.15496648289377
H	37.33385831860464	-23.41462301386432	2.65296517664278
H	37.26077166441230	-24.73836084740557	6.63907826106808
H	35.41330347607150	-25.08199408721483	2.89902553163913
H	32.25310226355898	-26.74003560905994	1.93833979993558

H	36.79824903866236	-26.76786510942353	9.67881747925714
H	37.51792040655344	-29.65208909412652	4.04596750867894
H	32.34741246825247	-23.00241854800247	7.10068458822562

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B3LYP Scan/Melmid IPC Model/BSS/70 degrees Constrained Optimization

C	38.90535007054331	-22.79257960053307	4.92578541448378
C	37.74212067877868	-23.70948148675834	4.73214133904335
C	37.07471296920444	-24.54687099554421	5.58978319207048
N	37.09005942082049	-23.86617934623912	3.51698018184819
C	36.08437616781999	-24.76804937053251	3.68733421124796
N	36.05218024537479	-25.19538946642150	4.93030885688651
C	30.57663361819952	-24.64415817209150	2.37781218166318
C	35.6409553082856	-24.65095604211328	10.93026621741468
C	39.10904163322139	-30.05836923352521	6.21301597957480
C	33.63065934816984	-28.65533259195066	0.57234415342410
N	33.16290506213056	-25.50468843119809	4.96344359071180
N	34.60169587910772	-25.51873476239178	7.42587808450217
N	34.79602460198124	-27.64328489752831	3.99745769902100
C	32.86688014068538	-26.68042773447998	2.83515145511867
C	32.88852655048142	-23.89170934994577	6.78509636516129
C	36.32067897441211	-26.69867321078672	8.70872200814173
C	36.80986017009209	-28.95180506824344	4.46211301408840
C	30.64694197964178	-22.71649451942938	5.00139355309611
C	33.40049686954556	-22.69835475924366	9.59934847132543
C	38.70267824036545	-28.63365683888309	9.11198241068048
C	36.36088911739906	-30.08602862278771	1.60875453408586
C	32.52417277376054	-25.70612330074064	3.76848093048221
C	33.82385565653033	-24.41844509270193	7.67074041085469
C	36.76053151540826	-27.56805227579997	7.71508411068327
C	35.75616550588930	-28.55352145332773	3.64543946317797
C	31.47671976327949	-24.71408697920328	3.57603403505065
C	34.07588738629191	-23.90025678472927	9.00733232200121
C	37.90038308960180	-28.46243755212937	7.85599900879730
C	35.50450995284871	-29.07254125850146	2.30970765935476
C	31.50740593808092	-23.90200083291459	4.67810394470724
C	35.01615880568467	-24.72244243851394	9.56826664118612
C	38.07016870316352	-29.06328894939739	6.63825186350039
C	34.35800461626355	-28.46589542338848	1.87023553971826
C	32.56302747694618	-24.41646600101812	5.53747307461478
C	35.33965794678419	-25.72210585449419	8.56078763111795
C	37.01657422035418	-28.54747347105147	5.77660066730994
C	33.93846174873467	-27.56383169749465	2.93208030334778
N	36.24281139459220	-27.64374578905811	6.45036475814992
Fe	34.63042542340172	-26.65244306116050	5.75219195257214
C	34.12328763007488	-31.47646012558752	6.68198084993255
C	34.92603120590150	-32.01619207751934	5.51025349427550
C	32.17944878818687	-27.48818669185582	7.20626719684164
C	33.40410896509070	-27.84633236861546	6.41315958156895
C	33.36945065797705	-29.29896482357034	6.07419238187802
O	32.58686505138758	-29.77819281460422	5.28208408546006
O	34.23172822115879	-30.03907036865469	6.81002847100405
H	29.92522184202376	-22.51322613916154	4.20395247367003
H	31.24372258543415	-21.80540735881418	5.14312412678921
H	30.07525271529994	-22.87108398342784	5.92637737570932
H	31.14508239987774	-24.50878718941327	1.44765496657746
H	29.98631543755420	-25.56277935179504	2.26051922928061
H	29.87178605813400	-23.81033769556619	2.45306169203360
H	33.45622111479179	-27.70084186985878	0.05833390144284
H	34.19348485775544	-29.29675757104950	-0.11310389814104
H	32.64812050880268	-29.12110758116908	0.72616919924116
H	36.03207863141146	-30.24255014711249	0.57653855873727
H	37.41344236610340	-29.77502180798305	1.57374124661172
H	36.33209680237518	-31.06246599567708	2.11115890744904
H	33.78084833337821	-22.47880422998136	10.60187727990729
H	32.31491814520700	-22.84232106557964	9.68543400203381
H	33.55630029902614	-21.80155708185132	8.98478489320387
H	36.73124812714645	-24.53108520055258	10.87175447508734

H	35.45151466153249	-25.56260819812964	11.51265904685664
H	39.52904848990659	-29.33636577261780	8.96703287233736
H	39.13631004566815	-27.68355491334432	9.45243295783396
H	38.08731536174481	-29.01799652603784	9.93666293268887
H	38.66158044569728	-31.01750154206308	5.91883233779793
H	39.68592627015389	-29.69774605808403	5.35080065516204
H	39.82114011804183	-30.26619516409519	7.01802439363308
H	35.24960163048134	-23.80766715744478	11.50775810764196
H	39.75384676598345	-23.05748112774027	4.28060523780075
H	38.64603002602479	-21.74523329181335	4.71937444595249
H	39.24895174627574	-22.8489988320246	5.96271524051438
H	35.97553674564086	-31.72558892715631	5.59216768497484
H	34.86970956933683	-33.10988925600784	5.49428196214668
H	34.53229676333247	-31.63561315853868	4.56701234444694
H	33.06859544311087	-31.74108720405790	6.58553395940368
H	34.50284305131379	-31.85572212323813	7.63237046801923
H	32.11668852845569	-26.43035920422966	7.44456544709215
H	31.28190418073957	-27.78111087505350	6.64534887479921
H	32.15446429102983	-28.05822584926183	8.14727470001162
H	37.31930245660349	-23.39456389344507	2.65396726747457
H	37.26340474242650	-24.72533945553781	6.63795328727179
H	35.41317653633406	-25.07799023598423	2.90000006320388
H	32.27159371489380	-26.72492091093249	1.92871889358474
H	36.82876508075909	-26.74674785955213	9.66672578965281
H	37.50611198018754	-29.67708852866679	4.05298974620319
H	32.33350840880725	-23.01882272111187	7.11382326268398

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B3LYP Scan/Melmid IPC Model/BSS/80 degrees Constrained Optimization

C	38.92915433051262	-22.83108748675073	4.95291820005024
C	37.75202125100233	-23.72497207832026	4.73706979399095
C	37.07221199796871	-24.57358342769041	5.57372214219029
N	37.09809025396549	-23.84191671662620	3.51840154542626
C	36.07895729083590	-24.73252831117342	3.66646945349649
N	36.04053637232822	-25.19029183825426	4.89838426782553
C	30.60568333252257	-24.49826417958971	2.32566151425175
C	35.58254028209388	-24.81553560481780	10.92336791872521
C	39.08320207449824	-30.07148876289552	6.05317968820231
C	33.57980812603032	-28.54426553510295	0.46596066320679
N	33.14879636845043	-25.47148552068587	4.91473730827461
N	34.57550625393360	-25.56188287857427	7.38224105627233
N	34.76725686817102	-27.59892177416990	3.90279476812169
C	32.85473151180795	-26.58659880715736	2.75448797688692
C	32.87145528174862	-23.91022402471528	6.78035333673669
C	36.28928058758562	-26.78095089542678	8.63709711307604
C	36.75470591154942	-28.95455335712260	4.34624632324715
C	30.67192513864913	-22.64835937550930	5.00496678830163
C	33.34937587817656	-22.82265407475092	9.64200638263804
C	38.68274310666761	-28.71280966860615	8.98737850139814
C	36.26886081110668	-30.05697954338896	1.48967892649194
C	32.51999404475426	-25.62945060925522	3.70864469525069
C	33.79371745774668	-24.47241819161383	7.65834655971012
C	36.72980324313932	-27.62575621968625	7.62259323405260
C	35.70558194137573	-28.52682632186319	3.53946294341086
C	31.48942572140864	-24.61644918038206	3.53209526255045
C	34.03337948530781	-24.00103446706073	9.01391008239635
C	37.87142699703217	-28.52132541381610	7.74008298430463
C	35.44132912026378	-29.02560802259237	2.19842724693496
C	31.51908219272987	-23.83655821392484	4.65700594099849
C	34.97156557771272	-24.83979344320885	9.55356213407515
C	38.03632180283621	-29.09808598239858	6.50926261798083
C	34.31090853565140	-28.38677539849584	1.76586798570013
C	32.55787297770523	-24.39054285830506	5.51248599387344
C	35.30606386108475	-25.80314349367495	8.51530650110125
C	36.97553769270296	-28.56859403215025	5.66458441713036
C	33.91094844673652	-27.48912224158991	2.83936460462310
N	36.20690270056400	-27.67616238665993	6.35885749121987
Fe	34.60481240334592	-26.65154868062573	5.68036447602726

C	34.16779637931113	-31.38883645915907	7.14069339687236
C	35.31796240055915	-31.95322133161315	6.32498360465911
C	32.08464473216590	-27.52162052039892	6.99379745806702
C	33.38642114603788	-27.85858618868847	6.32444793805594
C	33.48327019632965	-29.33449335625412	6.13371672907562
O	32.93663359356472	-29.93494772614985	5.23543843397472
O	34.16403917145443	-29.94186259820303	7.13652298628789
H	29.95878892929892	-22.41518946275920	4.20800228295251
H	31.27945695045840	-21.74916167772311	5.17439680632566
H	30.09152925192120	-22.81933298977011	5.92161200247748
H	31.18774456812647	-24.34238561566887	1.40718134753674
H	30.00488299276517	-25.40483665059838	2.17282812298498
H	29.91090278087436	-23.65771994087223	2.41775684251978
H	33.42701684679153	-27.57995548866591	-0.03662770744776
H	34.12857950534929	-29.18968922100878	-0.22700652151751
H	32.58699883995874	-28.99003485217863	0.61342497954954
H	35.93931928551047	-30.19286970545600	0.45475351474205
H	37.33085415799017	-29.77923496677497	1.46127329066509
H	36.20644430128687	-31.03676901265462	1.98240317099024
H	33.72005464756811	-22.63734506162332	10.65500690888269
H	32.26350059747836	-22.97242666727221	9.71307482423987
H	33.50803339286900	-21.90414392350212	9.06111603786295
H	36.67380951163545	-24.69838660386296	10.87980221324625
H	35.38361776494395	-25.74513001437249	11.47335897760592
H	39.50583756595013	-29.41596366343093	8.82662062933081
H	39.12151691442666	-27.76891247555394	9.33821923161174
H	38.07181018389681	-29.10674062363112	9.81074472749763
H	38.64415535540106	-31.02627903062120	5.73415023778046
H	39.65171125160405	-29.67980416436681	5.19906368691078
H	39.80107336211810	-30.29353997965992	6.84923291482250
H	35.18865203905874	-23.98999347060825	11.52434336219910
H	39.77435132833660	-23.09480791902712	4.30291443734544
H	38.68674696266967	-21.77538888174735	4.76990829179726
H	39.27023818615422	-22.91633416083436	5.98871163403359
H	36.27185240162051	-31.55901066073176	6.68184782929442
H	35.33677652305357	-33.04499112894989	6.41005809544553
H	35.20666742390200	-31.69046552578012	5.27184008410905
H	33.20715842754682	-31.74461088006095	6.76430543069479
H	34.26107357956601	-31.65300252027910	8.19573448932615
H	31.95085711028689	-26.45632841064390	7.16044081237222
H	31.25129065563495	-27.88925896954653	6.37863452648152
H	32.00669040285421	-28.04073181305638	7.96041189090827
H	37.33493821327581	-23.35304959060007	2.66713322832369
H	37.25732853960901	-24.78088893265299	6.61722411923436
H	35.40448539955285	-25.01443594096437	2.87146466021502
H	32.26433195670134	-26.60230863154212	1.84382818110913
H	36.79543542016359	-26.85437644855557	9.59448812772234
H	37.43720901969328	-29.68558397040444	3.92465444615277
H	32.31880958597112	-23.04479924588799	7.13198214452035

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B3LYP Scan/Melmid IPC Model/BSS/90 degrees Constrained Optimization

C	38.93915486706751	-22.83844757630223	4.96694070594758
C	37.75731323055630	-23.72353293713296	4.74100455901534
C	37.06719015642700	-24.57049942475792	5.57075764305004
N	37.11026366937798	-23.83272498376164	3.51793165575167
C	36.08505720590087	-24.71780847134508	3.65678898251109
N	36.03623770201351	-25.17907728483224	4.88702843641366
C	30.60903697536266	-24.46058787830570	2.30896524257309
C	35.56967380252929	-24.85987806554766	10.91314361487416
C	39.05737451237005	-30.09851881410510	6.00943117086876
C	33.57208208540907	-28.50437126614190	0.42596042208443
N	33.14238427738822	-25.46371281892756	4.89632087425639
N	34.56724105804498	-25.57500435261641	7.36411348012327
N	34.76788580234440	-27.57593194093698	3.86438192688155
C	32.85616912489064	-26.55443814051866	2.72289075629754
C	32.85715147011207	-23.92358990343797	6.77839176928382
C	36.28408993828698	-26.80110595984808	8.60836821605901

C	36.74354448194440	-28.94999135800263	4.30384841285224
C	30.66316506430789	-22.64314096978691	5.01043830019398
C	33.32934800272775	-22.86334558082909	9.65044838367715
C	38.67319451458004	-28.74009383236525	8.94712473250607
C	36.25020420773999	-30.03881225410460	1.44455795652642
C	32.51831712274225	-25.60742607009994	3.68617888474434
C	33.78061924081998	-24.49185785158617	7.65119590106366
C	36.72385844997697	-27.63951346064535	7.58837431872423
C	35.69937966410810	-28.50901354135230	3.49818938147582
C	31.48755420324123	-24.59333715204367	3.51765983335929
C	34.01814142934209	-24.03291028345048	9.01115548033886
C	37.86185371546654	-28.54026941422852	7.70100122301174
C	35.43201880306836	-29.00165751713269	2.15541870931604
C	31.51194717288877	-23.82709049219904	4.65203085002563
C	34.96006113931785	-24.87287145125185	9.54258906919366
C	38.02256298109742	-29.11372318422959	6.46785327487820
C	34.30596500793774	-28.35435294830733	1.72515504039947
C	32.54801396216439	-24.39028348643633	5.50460402351402
C	35.29861628889567	-25.82448126340034	8.49505183374523
C	36.96508090110035	-28.57468722896482	5.62533372488422
C	33.91119155505842	-27.45856916379228	2.80224821324597
N	36.20030668382900	-27.68224764193065	6.32432117830470
Fe	34.60084464982400	-26.64822393802317	5.65051266763005
C	34.14579058900555	-31.36004658480534	7.27027565018156
C	35.40596731560647	-31.89569302548351	6.61253794262687
C	32.08953583750210	-27.55482437312833	6.96138771625006
C	33.39358779037490	-27.86904389282634	6.28709246389474
C	33.54973375905220	-29.34454640234996	6.13338059731765
O	33.17260398687996	-29.97749927960134	5.17358799185269
O	34.08923925777439	-29.91454853401561	7.24036323219909
H	29.95175981218049	-22.40218415825589	4.21424924582937
H	31.26981208265031	-21.74537202530483	5.19040932779840
H	30.08075912524705	-22.82375441822580	5.92395805764627
H	31.19495862218509	-24.29292347177188	1.39503114727990
H	30.00927445157381	-25.36540301077974	2.14212541862169
H	29.91343109953665	-23.62159674316438	2.40867303936943
H	33.42531564034183	-27.53824541590782	-0.07499446479823
H	34.11519131625625	-29.15271335056351	-0.26869892789219
H	32.57633126937749	-28.94338583240123	0.57413226697561
H	35.92285274739210	-30.16567908126648	0.40777287561592
H	37.31548662799843	-29.77363295542342	1.42130506243363
H	36.17374604835764	-31.01999928446551	1.93239791859693
H	33.69839102962250	-22.68670807213929	10.66559554340224
H	32.24393186408263	-23.01747648805130	9.71897245610696
H	33.48540799438712	-21.93850885759170	9.07894056077564
H	36.66107713969406	-24.74347114908231	10.87171012504643
H	35.36915095514404	-25.79342819744527	11.45583802316074
H	39.49128726954704	-29.44853273934903	8.78403903916391
H	39.11879919434064	-27.79988732282954	9.29925430057000
H	38.06068572371829	-29.13139771385286	9.77054839618055
H	38.60540243869593	-31.05088783733608	5.70096886669541
H	39.62253010138616	-29.71819990605746	5.14813441270345
H	39.77946068618630	-30.32229911318708	6.80121145650400
H	35.17597179947936	-24.03854758804638	11.52001530575498
H	39.78771183070805	-23.10839487208771	4.32389425369853
H	38.70626966134077	-21.78090887030016	4.78237590990296
H	39.27095965196368	-22.92668672140546	6.00549478017466
H	36.29561075105605	-31.45999347158179	7.07218401891986
H	35.45122866328316	-32.98419707900401	6.72521310450752
H	35.41470189920572	-31.65757383131190	5.54808014042909
H	33.25138514409818	-31.75682007900400	6.78664678230653
H	34.11824128643548	-31.60555753420866	8.33355633930145
H	31.93264728721525	-26.49041892053499	7.11419987566188
H	31.25695056330416	-27.94687156666764	6.35902472681310
H	32.03327692996875	-28.06361526102295	7.93424429809441
H	37.35551935420478	-23.34293667579697	2.66959370666394
H	37.24429285289879	-24.78213029152120	6.61475881518142
H	35.41436917344264	-24.99402996880380	2.85663634705923

H	32.26757156180910	-26.56165907896474	1.81092464993684
H	36.79061979156644	-26.88112865494416	9.56502164771038
H	37.42064426151811	-29.68395928644683	3.87868605681451
H	32.30124762514389	-23.06388720200248	7.13880234935721

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B3LYP Scan/Melmid IPC Model/BSS/100 degrees Constrained Optimization

C	38.94158592475987	-22.81650690191368	5.07711885427530
C	37.77082025205690	-23.70651163710173	4.81561639961935
C	37.07487857862152	-24.57507286729292	5.61775394166191
N	37.14226521015269	-23.79502600426909	3.58122098950696
C	36.12149218740322	-24.68967421504605	3.68720768145824
N	36.05797448445033	-25.17619572108398	4.90704291557123
C	30.67333087405520	-24.42990322325173	2.23959869572032
C	35.48191630796214	-24.92340518645898	10.92482642982333
C	39.02587099427079	-30.14389177155543	6.04004246153856
C	33.70824165386696	-28.41088938058862	0.34321582543562
N	33.16206429869600	-25.45976739864764	4.85930103124489
N	34.54397102512742	-25.59799489189583	7.35049818642467
N	34.80837130941282	-27.55727617265421	3.83284358819136
C	32.92278772906422	-26.51821727847276	2.66439909405847
C	32.84335208718019	-23.94082151296354	6.75324769933881
C	36.23374682131188	-26.84241846829885	8.61418663502559
C	36.76840943385491	-28.94596630415345	4.29619758279678
C	30.67152542320762	-22.64891332874758	4.96568719605970
C	33.26805119575550	-22.90956300630602	9.64310690841661
C	38.60650501012636	-28.79880027518203	8.97858406131723
C	36.35826835417647	-29.96751593989563	1.40237760735817
C	32.56106027570637	-25.58862545480380	3.63575959204820
C	33.75364210461029	-24.51688723373596	7.63490617904583
C	36.68692123057148	-27.67517746525012	7.59547185108881
C	35.74839581594010	-28.48393883903665	3.47256040341427
C	31.52994479292839	-24.5758885506859	3.46240524407570
C	33.96762733042342	-24.07244931922948	9.00346832659736
C	37.81668923697357	-28.58446471228146	7.72100810314089
C	35.51786779071850	-28.94831857340905	2.11313321509337
C	31.53134870504072	-23.82470751211773	4.60705551323765
C	34.89876009586716	-24.91940022177668	9.54279725477567
C	37.99512023076047	-29.14964067420864	6.48638759460257
C	34.40342895635088	-28.29245243565325	1.66665469249673
C	32.55464505581705	-24.39515798790256	5.47027230304887
C	35.25439650829079	-25.86076970679615	8.49188113607197
C	36.95931781369423	-28.59402724518306	5.62855958623943
C	33.97930306808691	-27.41982075159877	2.75180805250507
N	36.18602215021190	-27.70365528622800	6.32149828659616
Fe	34.60381480102824	-26.65461816894205	5.62640233579375
C	34.00763798008276	-31.36957772473284	7.29255467679717
C	35.33548876718701	-31.88360416004693	6.76153624903521
C	32.09447972187795	-27.55755147927214	6.94205349104351
C	33.38373373379171	-27.87516198271584	6.24132687072317
C	33.55030351354620	-29.35056104067617	6.09846905572394
O	33.31948698563340	-29.98352816494029	5.09395639990590
O	33.93091144691421	-29.92481269000381	7.27051171923378
H	29.96551651230222	-22.40761289407467	4.16478787597513
H	31.27022371151844	-21.74808669921785	5.15693197276879
H	30.08245158078884	-22.83976852417874	5.87276536069530
H	31.27503854338853	-24.23931927886124	1.34044350686629
H	30.08669295567571	-25.33762820643325	2.04457213820541
H	29.96709831821088	-23.60005146763549	2.34090477815734
H	33.59359470039495	-27.43506215727457	-0.14742861966230
H	34.26216119947322	-29.05814008430709	-0.34387469244467
H	32.70111061292957	-28.83500732206836	0.45285352132895
H	36.06112719061661	-30.07114166920278	0.35397343971661
H	37.42294040331601	-29.69932176285244	1.41548544989986
H	36.27081083266069	-30.95959891534343	1.86553824573702
H	33.61879610356095	-22.74431581695579	10.66661680598355
H	32.18157568336778	-23.06407351778620	9.69058263069111
H	33.43445177535438	-21.97860540567607	9.08466660651965

H	36.57504351938410	-24.81844900627993	10.90540110739068
H	35.26088797561390	-25.85894736796338	11.45607172035069
H	39.42541404083300	-29.50770038088136	8.82170870713085
H	39.04887654319295	-27.86317793365312	9.34658094726471
H	37.98025993512280	-29.19636380575408	9.78856393482934
H	38.56782667217433	-31.09290000933339	5.73002889169299
H	39.60225192110745	-29.77103789099081	5.18299068798556
H	39.73873070329341	-30.37210175217735	6.83886117621225
H	35.08525726877235	-24.10265202887673	11.53052060313317
H	39.80134755055899	-23.06487733155362	4.44028281132587
H	38.70155582160616	-21.75730395374161	4.91221060316484
H	39.25973414994142	-22.92418262259775	6.11808015329440
H	36.17006774145152	-31.43937125863332	7.30843830962008
H	35.38497220328228	-32.97199502622097	6.87408732545963
H	35.44607528066393	-31.64035252769424	5.70425102229629
H	33.17313824197372	-31.77403012070652	6.71655872542953
H	33.87469798889622	-31.62619907067658	8.34513874417803
H	31.92996880925829	-26.49177966961879	7.07440277997933
H	31.24634579611861	-27.97061638522517	6.37567873214079
H	32.07437738436906	-28.04467011489174	7.92660444333053
H	37.39589329524355	-23.28594426738562	2.74681805056617
H	37.23842808498709	-24.80722118471812	6.65957986613720
H	35.46380630884998	-24.95310482629237	2.87207290172730
H	32.35486520197673	-26.51163434353409	1.73941461060417
H	36.72283206559892	-26.93321072916778	9.57891145415468
H	37.45204489135186	-29.67627814018044	3.87531787719843
H	32.28075019825056	-23.08537175099298	7.11335657578613

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B3LYP Scan/Melmid IPC Model/BSS/110 degrees Constrained Optimization

C	38.93594538955467	-22.79331666890907	5.08469104363992
C	37.76842566530338	-23.68607329738723	4.81808137617000
C	37.07891055105537	-24.56566798063484	5.61379268256798
N	37.13630951730143	-23.76513122288802	3.58483575217986
C	36.11994967922556	-24.66540502244002	3.68515803446938
N	36.06252178703934	-25.16420928711617	4.90025834766440
C	30.66154510682774	-24.43704774182727	2.24220555505918
C	35.48646225263973	-24.94041026955559	10.91554529168950
C	39.02984854273517	-30.14722063669894	6.01662919791334
C	33.71091477647347	-28.40086508716418	0.32723901950461
N	33.16788183065038	-25.45789993076150	4.84834103067968
N	34.54796901948507	-25.60451286159459	7.33917393593780
N	34.82268280082275	-27.54129590607747	3.81143270993690
C	32.92647009604632	-26.51227374174421	2.65196093848908
C	32.84815538050132	-23.94484632851649	6.74733047475898
C	36.23545898669771	-26.85506730247246	8.60000390479104
C	36.78372235006634	-28.93033621144624	4.26980407542317
C	30.66372790568125	-22.65982417605931	4.97071403914210
C	33.27721027051636	-22.91910552544099	9.63834965382845
C	38.60410291335977	-28.81682848906888	8.96062550404452
C	36.37088442820276	-29.94790933330872	1.37721427147979
C	32.56275716177320	-25.58721557164858	3.62692381371079
C	33.75942334455073	-24.52277325214513	7.62649526784986
C	36.69051095522052	-27.68294289944126	7.57816574437021
C	35.76429523327681	-28.46462408072762	3.44794592352519
C	31.52558741283814	-24.57978810041480	3.46015412592843
C	33.97418710481602	-24.08206172680989	8.99594401406084
C	37.81876417067566	-28.59415375428419	7.70160568167511
C	35.53120616480918	-28.92901324799436	2.08898529613706
C	31.52818533647941	-23.83040972243732	4.60611940823686
C	34.90340387607261	-24.93242574004740	9.53344927848129
C	38.00064653162385	-29.15204603854182	6.46407334093076
C	34.41249221969238	-28.27790131043611	1.64685395720245
C	32.55731105222690	-24.39750131175793	5.46422612923448
C	35.25738317663421	-25.87168716179544	8.48014277602662
C	36.96957531244230	-28.58912125980385	5.60560834428147
C	33.98903262073465	-27.40720485663265	2.73390194468463
N	36.19351130789835	-27.70356272378968	6.30209639029731

Fe	34.61152274136521	-26.65237673467272	5.60882880608549
C	33.90751704155151	-31.39042946709592	7.29616620722831
C	35.29626968269460	-31.87893739163826	6.91777080184767
C	32.13299449393924	-27.56638514253646	6.97048755786678
C	33.39653499458492	-27.88424175522337	6.22422877857827
C	33.58187600493302	-29.35727050790695	6.08005535820595
O	33.49097020732837	-29.98245767630702	5.04873908757023
O	33.81293149926041	-29.94747879151853	7.28590466299733
H	29.95392402861470	-22.41990184910862	4.17277642890658
H	31.25861858419366	-21.75656075422073	5.16235702806488
H	30.07853716072107	-22.85585494578577	5.87920305835122
H	31.25698130485117	-24.24130921877163	1.34001220457678
H	30.07957142690416	-25.34818078765459	2.04910081018589
H	29.95058179453364	-23.61191720367237	2.34881991796989
H	33.59160525848660	-27.42654283586926	-0.16533586738800
H	34.26264597505043	-29.04876723441227	-0.36097552758126
H	32.70523963651691	-28.82679129729112	0.44319203392304
H	36.06727933193609	-30.05774261351962	0.33131113379388
H	37.43468784703793	-29.67593363088541	1.38234411275729
H	36.28950283774531	-30.93766912042614	1.84636785279904
H	33.63017483932219	-22.75541426589794	10.66135309770030
H	32.19065333427290	-23.07244836932455	9.68790550043779
H	33.44354814579317	-21.98769744517550	9.08067224383969
H	36.58020258183572	-24.84232809720278	10.89616070540478
H	35.25948883182247	-25.87450037873555	11.44686428258377
H	39.42287216570365	-29.52556812463100	8.80242449875654
H	39.04621809940057	-27.88377403897167	9.33543257516121
H	37.97492216059025	-29.21832345139359	9.76638166705075
H	38.57019738672776	-31.09502800680045	5.70541185037944
H	39.60710200580028	-29.77431788006310	5.16023202859221
H	39.74203668983572	-30.37761626062957	6.81539556273950
H	35.09501286471139	-24.11715802775779	11.52126321003863
H	39.79454435389926	-23.03080126549668	4.44216061643397
H	38.69019576601278	-21.73362130056597	4.93175355524986
H	39.25838308788791	-22.91033719034031	6.12331474417013
H	36.05581448839855	-31.42743398744057	7.56001305691969
H	35.35181203350521	-32.96745864698010	7.02572391323719
H	35.52148419069533	-31.62235425531053	5.88215240003365
H	33.15353752217889	-31.79645901688582	6.61886317705110
H	33.65377758308458	-31.66658747744140	8.32132398629689
H	31.91553793647824	-26.50239694413401	7.00401877647308
H	31.27198695124579	-28.08425203130315	6.52298633277807
H	32.21466147082173	-27.94020666053301	8.00035691427300
H	37.38503574997441	-23.24681867702338	2.75465078169107
H	37.24711888984005	-24.80766129815014	6.65265305883186
H	35.46086181256461	-24.92402741354494	2.86961412762821
H	32.35476823402486	-26.50755503560963	1.72929731204956
H	36.72268838461054	-26.95053199154807	9.56521354251072
H	37.46809989242917	-29.65816431571816	3.84588759924688
H	32.28491544733118	-23.09106550005355	7.11034985969795

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B3LYP Scan/Melmid IPC Model/BSS/120 degrees Constrained Optimization

C	38.93313088204138	-22.78964763970782	5.08550252938295
C	37.76629099189903	-23.68199223193151	4.81438938035950
C	37.08250160365444	-24.57276222585053	5.60266452935041
N	37.12807139995987	-23.74718782638549	3.58346101464430
C	36.11393525544413	-24.65058830791521	3.67790370144240
N	36.06355511874342	-25.16439249609691	4.88704648763489
C	30.65357763325173	-24.43015723415264	2.24000062667464
C	35.48932495921838	-24.98902294607705	10.90269327213553
C	39.04406622618380	-30.14378256771477	5.95938033939881
C	33.72665031432312	-28.35594542797060	0.28299914345145
N	33.16704913623096	-25.46410227187009	4.83395156023317
N	34.54931361264426	-25.62726881207118	7.32221889275642
N	34.82554900360887	-27.53312701436212	3.78023527299616
C	32.92494042291059	-26.50194750325228	2.62999309845868
C	32.84948171071095	-23.96304918384958	6.74298912877172

C	36.23737467509424	-26.88696500315005	8.57386186225074
C	36.79404070755523	-28.91688984653608	4.22389912891654
C	30.65992878213403	-22.66970420963983	4.97935848063766
C	33.28054691004611	-22.95771784966154	9.64042803889397
C	38.61333830420728	-28.84364925947710	8.91577947750594
C	36.39482821236677	-29.89825101204233	1.31948735948568
C	32.55962865833033	-25.58608316342632	3.61285423665916
C	33.76121038834031	-24.54732028528376	7.61743644264305
C	36.69330435934475	-27.70628851512117	7.54542271159627
C	35.77357127331278	-28.44603247434018	3.40723778110220
C	31.52054695453115	-24.57936963537079	3.45506157226175
C	33.97686611809355	-24.11634374959433	8.98957469652580
C	37.82609099798093	-28.61290325107344	7.65939600423794
C	35.54605662143602	-28.89491840040862	2.04240595583245
C	31.52503701531831	-23.83688112762357	4.60556100968458
C	34.90577976759452	-24.97108953472997	9.52090073410440
C	38.00960823858237	-29.15850206080744	6.41663973244054
C	34.42323790398863	-28.24662477213761	1.60649568110665
C	32.55674155729877	-24.40788613965119	5.45772005152314
C	35.25907700610353	-25.90299846162804	8.46112948852044
C	36.97516768177842	-28.59300051041632	5.56422800816124
C	33.99237899480472	-27.39196097368422	2.70341346733451
N	36.19435551878438	-27.71852582560728	6.26978300119876
Fe	34.61054344216411	-26.66323274248346	5.58493710569997
C	33.81037937964697	-31.38741837605805	7.37549725985964
C	35.26163809017769	-31.82096469804004	7.24571965973527
C	32.13595177760938	-27.57178153453051	6.95688238371054
C	33.39364447535598	-27.90052802703037	6.20534956446833
C	33.60866161587712	-29.37215482197502	6.10020630396982
O	33.68824095827516	-30.01251204978620	5.07739476189229
O	33.66979028363527	-29.95031580069046	7.33658841798814
H	29.94885865990712	-22.42515859982167	4.18398583205520
H	31.25422028875120	-21.76716597374385	5.17617048683180
H	30.07618582384149	-22.87243781673655	5.88730267915626
H	31.24618965927857	-24.22237422152713	1.33860218295608
H	30.07661964377299	-25.34281487839774	2.03937135109731
H	29.93799049992545	-23.61027932037765	2.35568756273267
H	33.60538055510827	-27.37596200077221	-0.19773738355737
H	34.28360424333238	-28.99289518871605	-0.41121488929688
H	32.72217720881518	-28.78724080649295	0.38934138425689
H	36.09346047260595	-29.99808449433292	0.27192696436463
H	37.45631237436714	-29.61747074213343	1.32921464445232
H	36.32091758308587	-30.89384862312614	1.77717302585040
H	33.63535009138673	-22.80014106018066	10.66374891108357
H	32.19417538845848	-23.11197120705318	9.69106973777501
H	33.44542865724180	-22.02281920560773	9.08821563058540
H	36.58323720274270	-24.89293584913426	10.88337127177990
H	35.26075913883925	-25.92602732116668	11.42813085207621
H	39.43315291570330	-29.54970350897308	8.75125194535340
H	39.05418136335656	-27.91267005199432	9.29722501306386
H	37.98590336975047	-29.25235901055975	9.71936141748268
H	38.59032888575273	-31.09222670299724	5.64162658547381
H	39.61688893993016	-29.76020293870487	5.10474311509859
H	39.75941174083945	-30.37564078340446	6.75481940740148
H	35.09978532805008	-24.16885751463592	11.51380737883051
H	39.78832978482342	-23.01658439802534	4.43466544147930
H	38.68368891025519	-21.72874183500930	4.94764302612252
H	39.26237774461139	-22.91905262603339	6.12050514414917
H	35.88052534037820	-31.34145151579623	8.00764830792615
H	35.34148735786378	-32.90667685160442	7.36550593803960
H	35.65419897158303	-31.55188496931308	6.26461502821350
H	33.20019457524410	-31.82325018866383	6.58225022151586
H	33.39460797357770	-31.67177666286378	8.34412128000441
H	31.89867600543942	-26.51168724329563	6.94305231409502
H	31.27574378067683	-28.12611789699103	6.55404735262743
H	32.24332019282229	-27.89310653935759	8.00148740934838
H	37.37159470391430	-23.21807703088390	2.75854835301837
H	37.25593584380232	-24.82691138947936	6.63777146690636

H	35.45128220085515	-24.90028832526885	2.86246295736157
H	32.35299493579716	-26.49115178406056	1.70753521373562
H	36.72572947068846	-26.98834844970086	9.53787623755027
H	37.48220628561922	-29.63617968522155	3.79180386710322
H	32.28639793161017	-23.11197307962750	7.11244967626088

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B3LYP Scan/Melmid IPC Model/BSS/130 degrees Constrained Optimization

C	38.94383791304358	-22.79205085106445	5.08189103441934
C	37.77302483760172	-23.67708245187837	4.80397881869996
C	37.09896226542447	-24.58709635287599	5.57863956586542
N	37.11871937764846	-23.71126288396081	3.58018333495646
C	36.10513290688135	-24.61624495729841	3.66550600633180
N	36.07030069781258	-25.15995818436182	4.86196220016241
C	30.65355046502545	-24.40690368665251	2.23018204651590
C	35.46655244364966	-25.09520376193277	10.89238693481360
C	39.07316486573049	-30.12981092706994	5.85882186446911
C	33.73000096054783	-28.30528612982268	0.22371541687455
N	33.17356620364176	-25.46837865019890	4.80680171699018
N	34.55659058577071	-25.66120934035562	7.29252962021751
N	34.82931608671480	-27.52144019200443	3.73008056776399
C	32.92419436124368	-26.48335489091583	2.59333100914330
C	32.85181612230578	-23.99419218063701	6.73636891968595
C	36.24326719918922	-26.93851855782452	8.52979578514347
C	36.81192963326797	-28.89341044069353	4.14827252913104
C	30.66612300238519	-22.67534883427231	4.98790300413610
C	33.25752901640741	-23.04769344060883	9.65647732619532
C	38.63403923878700	-28.88565649066919	8.83832653362465
C	36.41062603967528	-29.84293264747256	1.23548744612235
C	32.56272917668638	-25.57697772413286	3.58622828213478
C	33.76051412080540	-24.59176979326414	7.60457529363517
C	36.70587981884417	-27.73761180296031	7.48849784889851
C	35.78387534358523	-28.42211913423387	3.34285368512178
C	31.52344993501834	-24.56873146865927	3.44152266921484
C	33.96534550880418	-24.18808650397612	8.98609581637234
C	37.84528890235567	-28.63778163210656	7.58643243311160
C	35.55596978497230	-28.85557444140392	1.97336302757322
C	31.53036055872170	-23.83859254848874	4.59999919098732
C	34.89513228860171	-25.04929081416956	9.50617555773552
C	38.03138033126230	-29.16087029278276	6.33448741895811
C	34.42716361832606	-28.21028103847705	1.54810459629503
C	32.56333017273991	-24.41916739614128	5.44386249562719
C	35.26071635555544	-25.95705986274911	8.43036700899808
C	36.99199368477618	-28.58877816551487	5.49258999089439
C	33.99366434773912	-27.37145188178935	2.65589695880534
N	36.205466889292861	-27.73241365063568	6.21306941077094
Fe	34.61727808634932	-26.67383324246558	5.54499736749369
C	33.72347808555016	-31.34915734715295	7.53086630242440
C	35.18583611677004	-31.70300256957308	7.74920650471421
C	32.13334873887446	-27.57147343146207	6.90373363853892
C	33.40356800763511	-27.91955981609232	6.18041999801791
C	33.67381617028090	-29.38350128426616	6.15958044809511
O	33.95037647008555	-30.05549574567624	5.19248182079683
O	33.53290061890450	-29.92420128192655	7.41023707270642
H	29.95419107267462	-22.42205162552210	4.19608856775972
H	31.26114415471244	-21.77532032497278	5.19371308600309
H	30.08336538087597	-22.88769398486306	5.89426053641190
H	31.24434775951038	-24.19498105034877	1.32859209560465
H	30.07212855640975	-25.31563984294681	2.02465112508379
H	29.94178879415185	-23.58493076182762	2.35413329766093
H	33.61911309072801	-27.32140736276394	-0.25174314300948
H	34.28089786249176	-28.94393063404318	-0.47369369852546
H	32.72100825005398	-28.72664447833538	0.32683506465627
H	36.10325860488831	-29.93651702088835	0.18910872217367
H	37.46893467451024	-29.55030129447598	1.24075896936802
H	36.35091482398701	-30.84315194277019	1.68488969447702
H	33.59863236841561	-22.91455511317398	10.68787236179836
H	32.17118899671545	-23.20642171488432	9.68940809417210

H	33.42636616741319	-22.09882578630835	9.12989122824075
H	36.56106259715095	-25.00546827080855	10.88434287762011
H	35.22764499463771	-26.04011843909958	11.39875253095227
H	39.45957239348352	-29.58181774307113	8.66089971358666
H	39.06709410659199	-27.95842431021946	9.23728860226316
H	38.00991516823397	-29.31466725709414	9.63385366798029
H	38.62527320046182	-31.07072336235689	5.51208781870941
H	39.65057457861929	-29.72102415260860	5.01900834808749
H	39.78336477535300	-30.38021604771768	6.65314707907970
H	35.07650808285618	-24.28377423166496	11.51470262660456
H	39.79035520656870	-23.00293545211129	4.41450715779186
H	38.69314790636728	-21.72801782394776	4.97365744613115
H	39.28648302131491	-22.94715605466330	6.10897435934737
H	35.58579360980058	-31.17733303571957	8.61980505425605
H	35.29274610226106	-32.78008085099039	7.91642629092052
H	35.78209174266571	-31.42834486195707	6.87786047801547
H	33.33236249205979	-31.83583587529304	6.63585493007710
H	33.11284448790171	-31.63350749952629	8.39027410893567
H	31.79086497094504	-26.56257315735995	6.68864619032256
H	31.32280368465602	-28.27574961893994	6.67540827985717
H	32.30561855588331	-27.64341159555863	7.98643763448565
H	37.35179205787692	-23.16162876520756	2.76573257727784
H	37.28561465487066	-24.86743575569687	6.60468090326630
H	35.43117242098585	-24.84467711190105	2.85304385845736
H	32.34998410630769	-26.46398957174054	1.67245416091321
H	36.72924959632370	-27.05383178374639	9.49341649873896
H	37.50348437745203	-29.60227702789290	3.70473132117274
H	32.28501017690407	-23.15112477531057	7.11821666408980

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B3LYP Scan/Melmid IPC Model/BSS/140 degrees Constrained Optimization

C	38.92740031701378	-22.75678399560584	5.08369297295766
C	37.76513008037747	-23.65185719660730	4.80209529248244
C	37.10160406154151	-24.57339714490653	5.57214875954909
N	37.10901274528791	-23.68491594643478	3.57918375872289
C	36.10438232751501	-24.60010675755674	3.66065222983209
N	36.07708597938378	-25.15149476053495	4.85380670733901
C	30.62879287508598	-24.44808089992591	2.24427984928143
C	35.46696359771852	-25.11134893185540	10.88887180769726
C	39.09403589808702	-30.11858766332648	5.84207200376953
C	33.74820363584644	-28.30299050974808	0.21390794715092
N	33.18165153949214	-25.47563601122521	4.80146782301551
N	34.57168310828936	-25.66229493692238	7.28344588185333
N	34.84792790663587	-27.51365088254959	3.71876914678016
C	32.92319836062192	-26.50050959122613	2.59354605228741
C	32.86651470439565	-23.99547443849994	6.72773516515936
C	36.24651950669696	-26.95184200384043	8.52393047335224
C	36.85119715243221	-28.85802493700915	4.12618582260857
C	30.65658329483685	-22.69962507128219	4.99145243677629
C	33.27180387014121	-23.05116324946155	9.64911178099698
C	38.62347892104629	-28.91755587397875	8.83477774124210
C	36.46314529663988	-29.79232510800547	1.20715871380960
C	32.56055326980060	-25.59513501433402	3.58699988784834
C	33.77740262037928	-24.59128139567274	7.59499162656304
C	36.71441039955912	-27.74384388733736	7.47952254487400
C	35.81738515768384	-28.39480358614029	3.32389680051440
C	31.51261510736533	-24.59556044170857	3.44737089311641
C	33.97891869102352	-24.19159626759140	8.97802747898080
C	37.85016583795026	-28.64897006366766	7.57760090250389
C	35.59251719301179	-28.82507550164258	1.95300216438966
C	31.52616394000121	-23.85814703079820	4.60142920407253
C	34.90244168721055	-25.05869247928407	9.50006159682911
C	38.04957547716693	-29.15373114438473	6.32012117521399
C	34.44914805957731	-28.20021009537249	1.53571742057376
C	32.57051041828672	-24.42699914849188	5.43895856192620
C	35.26936572271914	-25.96475782524959	8.42339747059100
C	37.01961166901854	-28.56889670024994	5.47528332007269
C	34.00544657079752	-27.37350429801721	2.64883345317253

N	36.22683901586512	-27.72218455929804	6.19932776839009
Fe	34.63372808887923	-26.67185386546898	5.53501357008559
C	33.62100210641687	-31.38240943341507	7.48649475150407
C	35.06276956445267	-31.70385923039328	7.84915034555376
C	32.18008712655596	-27.55864616657437	6.94942255767886
C	33.42090134663700	-27.92588756736223	6.18524959876616
C	33.69077098904087	-29.38768204616495	6.15829295414140
O	34.09538102407244	-30.03914780113610	5.22196076458788
O	33.40435173973382	-29.96194351490569	7.37170850579273
H	29.94433057545529	-22.44731567857053	4.19961609275756
H	31.24750439476543	-21.79765805381445	5.20018844833371
H	30.07377387304439	-22.91690240382724	5.89667758199911
H	31.20891061802276	-24.24349790673567	1.33413840827019
H	30.04798042074966	-25.36060841937775	2.05428094275587
H	29.91579406821293	-23.62715002888322	2.36795184240148
H	33.62460653199121	-27.32045654952529	-0.26127541556784
H	34.30373649758852	-28.93552618237406	-0.48541141708588
H	32.74439245765144	-28.73560538098037	0.32063563052531
H	36.14996245030935	-29.89166143700595	0.16305222539513
H	37.51476546916304	-29.47635666180151	1.20503663944218
H	36.42899502779581	-30.79401732941790	1.65596436508445
H	33.61428638953117	-22.91771407776075	10.68000575098040
H	32.18553498572582	-23.21023841974100	9.68359997367997
H	33.43967770038302	-22.10245849386895	9.12201490768642
H	36.56155926524598	-25.02216670339546	10.88668785645265
H	35.22505274580966	-26.05850026174480	11.38955076758627
H	39.45351834437773	-29.60783758916737	8.65540251522662
H	39.04826803202371	-27.99649611370435	9.25621973899936
H	37.99018424891096	-29.36307662563564	9.61381355004060
H	38.64731500083667	-31.05506606566827	5.48222835336391
H	39.67803498038929	-29.70153532404144	5.01093323608024
H	39.79814111861025	-30.37794913613866	6.63894429370440
H	35.07410846948717	-24.30274938141472	11.51310677453765
H	39.77531452388239	-22.95555057507390	4.41437557402136
H	38.66590047895758	-21.69476041267987	4.98149091031884
H	39.27256569627826	-22.91398016010031	6.10960954378161
H	35.35838817876105	-31.17842948646429	8.76101424102222
H	35.17947037664259	-32.77971012189875	8.01769903126656
H	35.73787281043500	-31.40583923192364	7.04571952024048
H	33.33714906736023	-31.86279443403703	6.54851499154011
H	32.93392777556766	-31.69928546240513	8.27391263568284
H	31.81660085552198	-26.56505847527239	6.69893901183776
H	31.36975093425446	-28.28214516161060	6.79943197129991
H	32.40219776132278	-27.56672820991033	8.02545781632216
H	37.33496061541788	-23.12766821545087	2.76789437324470
H	37.29286718970549	-24.85836025657286	6.59606413890494
H	35.43076912206743	-24.82971305486844	2.84823722471405
H	32.34189555556934	-26.48949612264439	1.67698767198935
H	36.72470548631962	-27.07629399555464	9.49031377273410
H	37.55210810421350	-29.55489664006938	3.67833979869145
H	32.29956078434957	-23.15259687670358	7.10977072533106

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B3LYP Scan/Melmid IPC Model/BSS/150 degrees Constrained Optimization

C	38.93014318282990	-22.72703250618417	5.05863197913152
C	37.76640195457144	-23.62265292622606	4.78492293669726
C	37.11828732114332	-24.55611409928752	5.55383551089352
N	37.09125192768902	-23.64305929036054	3.57208139306412
C	36.09146398907185	-24.56317955700464	3.65784580200527
N	36.08503215156917	-25.12925637257359	4.84429735611271
C	30.60421063928624	-24.48998500463675	2.26894783594816
C	35.48748256930359	-25.12900892862566	10.88520369573191
C	39.14349588715437	-30.08037824412645	5.80449892740935
C	33.76079944435949	-28.30321016259831	0.20918493697710
N	33.19192153873178	-25.48791615848819	4.80264635407181
N	34.59268057862135	-25.66973912640066	7.27829372483160
N	34.87276753425786	-27.50199240678839	3.70747980381944
C	32.92347935058983	-26.51817568545889	2.59873282004180

C	32.87942387415320	-24.00848783776271	6.73028057800388
C	36.27061094731368	-26.95988416320869	8.51312225768133
C	36.90467145036721	-28.80824169128332	4.09540509200593
C	30.64722852595111	-22.73109888347986	5.00931207190126
C	33.28797114886601	-23.06920567511573	9.65295621908221
C	38.65033861949697	-28.92394743304028	8.81240446179040
C	36.51688758981972	-29.73471756841328	1.17372647387580
C	32.55999793766507	-25.61567330775376	3.59452409870558
C	33.79511411625188	-24.60194932562323	7.59387095868298
C	36.74478660426316	-27.73919582704008	7.46205145514694
C	35.85864981416499	-28.35971978050386	3.30104726401728
C	31.50220376826928	-24.62580972907303	3.46293846266966
C	33.99697431002500	-24.20603291016462	8.97769105380481
C	37.88350693655624	-28.64168176783464	7.55422004960518
C	35.63276930790169	-28.78793791312272	1.92996573193167
C	31.52196088800266	-23.88410998179423	4.61443914740929
C	34.92234982404535	-25.07321753915340	9.49673026195842
C	38.09304903493532	-29.12623942435599	6.29043393564750
C	34.47190274736439	-28.18726143618540	1.52458578454076
C	32.57819773347785	-24.44250798107070	5.44347401630200
C	35.29133164701800	-25.97435171631488	8.41698273787148
C	37.06467891602627	-28.53463338883481	5.44839277801621
C	34.02006534402008	-27.37379291273715	2.64390719584126
N	36.26329442414153	-27.70330418191794	6.18014184982484
Fe	34.65860477795519	-26.67153841488572	5.52703687366379
C	33.48807335841148	-31.43692837311434	7.40350157845704
C	34.81003135694002	-31.70986904942033	8.10506513472854
C	32.20034492620994	-27.57453639394123	6.92625367911316
C	33.45098791968799	-27.94434388765889	6.18055381690610
C	33.73486940157790	-29.40165064694281	6.15723660297994
O	34.30997324257380	-30.02228974312312	5.29050646536452
O	33.24499993893448	-30.02294243449870	7.28270768526897
H	29.92483054544663	-22.48755536602801	4.22397284810967
H	31.23314203617212	-21.82365568805539	5.20824339555339
H	30.07560205061899	-22.94918935890196	5.92140903470300
H	31.17161647549138	-24.27531088733736	1.35310436032522
H	30.03534235869628	-25.41091733772162	2.08365746036899
H	29.88006297713184	-23.68020400188006	2.40113329494138
H	33.59149181886597	-27.32119601048687	-0.25240833201402
H	34.33379429786912	-28.90424957653856	-0.50376616642847
H	32.77681107757668	-28.77810826563860	0.32153031556098
H	36.20004344727700	-29.83349398490226	0.13066061425079
H	37.56252262259279	-29.39964985578036	1.16843597914717
H	36.50325822511177	-30.73952916562996	1.61666858147549
H	33.63051268956061	-22.93876112707341	10.68421139573281
H	32.20202553358725	-23.23040625574087	9.68727928744634
H	33.45399017481357	-22.11836966133793	9.12913574454202
H	36.58216351352446	-25.04144631292721	10.88259219574488
H	35.24438389060132	-26.07661136303765	11.38450478572051
H	39.47681012215585	-29.61811371840151	8.63137157359663
H	39.07949771271073	-28.00842848643823	9.24162600058195
H	38.01101939202172	-29.37060532631989	9.58568034515817
H	38.70036302365365	-31.00918422285771	5.42154895193918
H	39.73603623135988	-29.64646178232901	4.98809061527673
H	39.83927953242119	-30.35498571894235	6.60355654358505
H	35.09614061422599	-24.32085649005356	11.51095817958410
H	39.76736865004059	-22.91430948735244	4.37273961885296
H	38.66339910410461	-21.66475786015769	4.97427239382663
H	39.29304291802085	-22.89602370358827	6.07652129306209
H	34.83459280169669	-31.22290959093519	9.08360833591953
H	34.94769866613073	-32.78628229656999	8.25246865164368
H	35.64642833813888	-31.33488984906537	7.51194913917191
H	33.47063842969407	-31.88834251927205	6.41053246621465
H	32.64522584436197	-31.81508973605745	7.98629983556367
H	31.84477409141774	-26.57875922719192	6.67472991932239
H	31.39113653322855	-28.29481662139952	6.76079228940540
H	32.40232191998912	-27.58815544782999	8.00650251477109
H	37.30281769156279	-23.07521617966272	2.76425541379658

H	37.32634113220718	-24.85307181713229	6.57109954876521
H	35.40621149733697	-24.78549027761915	2.85313256922402
H	32.33433083636032	-26.51460225942024	1.68716301757497
H	36.74688482825742	-27.09062153241112	9.47960053798742
H	37.61615039989682	-29.48970938136008	3.64067861514131
H	32.30944443750075	-23.16919655348503	7.11565168532028

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B3LYP Scan/Melmid IPC Model/BSS/160 degrees Constrained Optimization

C	38.90951096836121	-22.67342770497259	5.02382229837559
C	37.75460224559922	-23.58463231785953	4.76451109543110
C	37.12243757954317	-24.51957905550628	5.54475617341526
N	37.07241980970699	-23.62279351429374	3.55604819994600
C	36.08425000148608	-24.55404306490818	3.65520328289919
N	36.09187041068469	-25.11075491163799	4.84606621098898
C	30.57591910752141	-24.56925920052004	2.31482857921359
C	35.54266793459750	-25.06418582199844	10.88926983161193
C	39.22488554469942	-30.00206729005561	5.81758966133698
C	33.76495055797901	-28.36528526201706	0.26166836217934
N	33.20364965447513	-25.50669416927841	4.83037205812838
N	34.62541990522825	-25.65017401796859	7.29525251811620
N	34.90091779695996	-27.50648550159937	3.73848024115622
C	32.91977605071245	-26.57050427656349	2.64458386289710
C	32.90465066564262	-23.99932547533468	6.73841436618377
C	36.31854614016226	-26.91779004945884	8.53089415098706
C	36.96866754547607	-28.75889364809063	4.11265516901712
C	30.64551636552682	-22.76195545176208	5.02285284984515
C	33.33420356019546	-23.02119969879156	9.64590703867267
C	38.71855907791107	-28.85740544076749	8.82777341168750
C	36.57013331763437	-29.71365107561960	1.19923872488152
C	32.55736772234796	-25.65900253093822	3.63255097666455
C	33.82860662839484	-24.57918535648974	7.60269300921899
C	36.79741684353807	-27.69475650444552	7.48001718557758
C	35.90404405164093	-28.34120476359697	3.32587956758539
C	31.49069873128621	-24.67921280107614	3.49878411381227
C	34.03927207364040	-24.16606510255053	8.98012909642553
C	37.94866454735278	-28.58188573179491	7.56999158059097
C	35.67262598856885	-28.78358545747077	1.96051580846717
C	31.52161001163545	-23.91689340191786	4.63669518274508
C	34.96830149581414	-25.02642954871267	9.50399936671152
C	38.16463433146849	-29.06015941509182	6.30529611270940
C	34.49094665598300	-28.21634823726167	1.56574534233719
C	32.59140409499412	-24.45473513538721	5.46148933726388
C	35.33243840437099	-25.93940823620428	8.43258523260089
C	37.12675041237259	-28.48288566216754	5.46513200719672
C	34.03278397396631	-27.40552026780691	2.68434304533696
N	36.31363618030009	-27.66525471950346	6.19940893134856
Fe	34.69116991324531	-26.66624030726706	5.55255248579283
C	33.24942853476248	-31.52004347859926	7.18637090032665
C	34.47732632984179	-31.90029143775283	8.00090485370968
C	32.23600929845815	-27.58301932814295	6.95187308188585
C	33.49198802023113	-27.95376044847374	6.21773874017337
C	33.75731204699171	-29.41275595870159	6.16415928731054
O	34.47677959109811	-29.99968548836060	5.38435171806054
O	33.06287933864982	-30.09409566341095	7.14003281702769
H	29.91347868907395	-22.53402838551501	4.24176636453707
H	31.22919460866695	-21.84876638938188	5.20095180073054
H	30.08489712956246	-22.96807014101902	5.94451540760566
H	31.12770208887205	-24.35086949212879	1.39027778764324
H	30.02224684550404	-25.50198982108942	2.14338772211655
H	29.83816435201336	-23.77229805585681	2.44988441121727
H	33.51368611185164	-27.39207109289083	-0.18000935293004
H	34.36733280146609	-28.91092114568137	-0.47153711155284
H	32.82171307422634	-28.91501200022569	0.38389751951835
H	36.25372795016307	-29.81225298176793	0.15595035990752
H	37.61058025860979	-29.36313455637053	1.19493488196218
H	36.57183185815548	-30.72086414976878	1.63712184430441
H	33.68890192867970	-22.87317921670260	10.67067161617274

H	32.24929322320297	-23.18548647038545	9.69606439122610
H	33.49049760296569	-22.07833096725086	9.10497766675661
H	36.63701900723538	-24.97317376756007	10.87834086375326
H	35.30598098535220	-26.00666706882275	11.40120866472796
H	39.54996455467752	-29.54563160109708	8.64664243573795
H	39.14143975489481	-27.93848021881844	9.25610967328613
H	38.08298349392600	-29.30793703266182	9.60186254000811
H	38.79009607212331	-30.93431967994692	5.43345448893689
H	39.81285027555587	-29.56090971463837	5.00170623518180
H	39.92362683071949	-30.27113023455146	6.61596838457568
H	35.15274350419988	-24.25009064151946	11.50818584413634
H	39.74410180257281	-22.85569835478794	4.33339145336191
H	38.62970301991591	-21.61496698510516	4.93394651797841
H	39.28147472523477	-22.83103885235119	6.04027690612816
H	34.41608651566975	-31.48533884707071	9.01070681871320
H	34.55644751979385	-32.98957907111904	8.08191476859016
H	35.38512235643110	-31.52521265372368	7.52520589049620
H	33.32445296858078	-31.90368245584333	6.16737033917228
H	32.33569726281440	-31.90177909196755	7.64715826827151
H	31.98370127150201	-26.53227620892655	6.84829342382896
H	31.38231397475588	-28.18521980322982	6.61689406132429
H	32.35004511661224	-27.80248363003786	8.02200866909572
H	37.27237200014127	-23.05897067948800	2.74244938417701
H	37.34038872485830	-24.80575256139505	6.56304265964462
H	35.39713476885172	-24.79119695938486	2.85633588440580
H	32.31918237717663	-26.58651102336093	1.74065835854954
H	36.80002122808143	-27.03978765131318	9.49594153729473
H	37.69316051872572	-29.42462379979130	3.65516766320328
H	32.33580837052604	-23.15607070632309	7.11673878835421

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B3LYP Scan/Melmid IPC Model/BSS/170 degrees Constrained Optimization

C	38.90195735992083	-22.64153212289546	4.99404135372384
C	37.75136376148311	-23.56136772678061	4.74638802753683
C	37.12408157839904	-24.48941315015370	5.53869313093888
N	37.06956223575875	-23.61894465787276	3.53851191370172
C	36.08653760588557	-24.55441838046040	3.64971428146885
N	36.09713650227975	-25.09547512743461	4.84765546122986
C	30.55902065461570	-24.62516243687741	2.34879690488898
C	35.57978495311659	-25.01665809804517	10.89555172288283
C	39.29122755084967	-29.93314536829644	5.82781043783811
C	33.76090860925679	-28.41717089213232	0.30825055219359
N	33.20923150182450	-25.52319935873852	4.85483627021699
N	34.64763854715643	-25.63608036163647	7.31101820862582
N	34.91775217381124	-27.51463827934980	3.76650218660289
C	32.91559960757915	-26.61195533152040	2.68275687607021
C	32.91730808524496	-23.99704830691391	6.74903056598831
C	36.35418373923979	-26.88405617950595	8.54621724158058
C	37.01195825697655	-28.72539045972847	4.12929632359216
C	30.64238593071481	-22.78631986682910	5.03481588528678
C	33.36025109471353	-22.99026114392345	9.64518183871682
C	38.77500306049959	-28.79705154504312	8.83915105598863
C	36.59725436309026	-29.71384674115367	1.22754610894625
C	32.55471231370958	-25.69212960962584	3.66363345564286
C	33.84887458889749	-24.56473736374990	7.61308872961615
C	36.83771092964249	-27.65772939710147	7.49499602540282
C	35.93110622954848	-28.33516604711695	3.35015227997224
C	31.48308578408199	-24.71842299054621	3.52696945361934
C	34.06478769647172	-24.13930674864855	8.98600934132656
C	38.00103028232588	-28.52920669408961	7.58226769469850
C	35.69251830946177	-28.79250313668627	1.99090744166870
C	31.51952382282981	-23.94290757428683	4.65596485697437
C	34.99845756528191	-24.99278734305636	9.51289475406429
C	38.22137286342288	-29.00321006574078	6.31698835479049
C	34.49751041470931	-28.24773016203584	1.60388627994350
C	32.59700716854884	-24.46729052680251	5.47907960790183
C	35.36105980927154	-25.91302248887898	8.44709896387331
C	37.17304565204255	-28.44155620858870	5.47954709527239

C	34.03808195576919	-27.43443305015870	2.72006189259865
N	36.35035595310305	-27.63522199251877	6.21610802404769
Fe	34.71268632403581	-26.66375172559662	5.57464329305546
C	33.09308665425560	-31.57128395494577	6.96528160559961
C	34.20546298566553	-32.02375500127933	7.90040345854977
C	32.27939518433773	-27.59075780965473	7.00209107499385
C	33.52213956601553	-27.96300624094949	6.24723960598479
C	33.77149437293144	-29.42150124959446	6.15597306360915
O	34.59889472420909	-29.98427226492726	5.46969184613155
O	32.93095285404063	-30.14205368429765	6.97796049105204
H	29.90868975605361	-22.56512514379916	4.25333442814013
H	31.22520348135603	-21.87113536063444	5.20516962690192
H	30.08342758332066	-22.98610128464947	5.95890625017201
H	31.10549070842404	-24.43682005929780	1.41465615749245
H	29.99139787398444	-25.55423918734083	2.20474468419341
H	29.83312340341685	-23.81529273075013	2.47062372703477
H	33.50910224601477	-27.45083890616965	-0.14826892301124
H	34.35585163780026	-28.97712973908544	-0.42012670580420
H	32.81689079727207	-28.96140333358476	0.44723532665698
H	36.25849664041520	-29.84423744674638	0.19486785135599
H	37.62722808965733	-29.33512746380514	1.19007054294679
H	36.63785484100750	-30.71052612093903	1.68698231731394
H	33.71859659793317	-22.83333836400264	10.66734542019493
H	32.27578480405423	-23.15571687531065	9.70073479990642
H	33.51305968390528	-22.05159034804317	9.09597550393542
H	36.67318532671917	-24.91534432424547	10.87871038308991
H	35.35466210457250	-25.95816757083400	11.41442025720604
H	39.61131408540462	-29.47923825259440	8.65778410265737
H	39.19143921359422	-27.87456634761877	9.26622129341190
H	38.14370631956824	-29.25151681256424	9.61445954561557
H	38.86561433481894	-30.87132594388293	5.44779849244790
H	39.87104158783190	-29.48728491203426	5.00865606276817
H	39.99593676168948	-30.19205010083579	6.62430751676782
H	35.18509973236291	-24.20254990788719	11.51140628473313
H	39.73709432794989	-22.82829997798178	4.30548444732196
H	38.61733004209461	-21.58550056813336	4.89169024906617
H	39.27517265856559	-22.78534544336394	6.01210105295071
H	34.02747003927982	-31.6657903322411	8.91814536919571
H	34.25676118568532	-33.11741791047478	7.92655669813731
H	35.16990226495017	-31.64324860935202	7.56039037665036
H	33.28926276861459	-31.89863295755355	5.94254811567864
H	32.12385311613510	-31.95902759180020	7.28629245232621
H	32.06313717133842	-26.52819809174417	6.95695756205878
H	31.40783357068208	-28.14355636954922	6.63026269614408
H	32.37835594044729	-27.87617611099182	8.05816409505187
H	37.26681520647851	-23.06486407659206	2.71758314622124
H	37.34365184399633	-24.76104298134185	6.56062622104274
H	35.40119064617099	-24.80585672012202	2.85367536997347
H	32.30732261943771	-26.64290510715292	1.78433081541513
H	36.84023371949363	-26.99877597338373	9.50987656345060
H	37.74508944868197	-29.38002925774335	3.66946156309179
H	32.34764162633855	-23.15212260967000	7.12239692168685

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B3LYP Scan/Melmid IPC Model/BSS/180 degrees Constrained Optimization

C	38.87552823518202	-22.59156318295237	4.95192502233904
C	37.73615588386755	-23.52978299096051	4.72201966947803
C	37.12988639164752	-24.46085160961930	5.52700903773614
N	37.04384709006108	-23.60607950347543	3.52123501292479
C	36.07542029098176	-24.55462625766978	3.64865935452565
N	36.10510198330195	-25.08663747489905	4.85033277126459
C	30.54130416708973	-24.70674888141086	2.39836808378696
C	35.64763971168846	-24.94942443765841	10.90023962724219
C	39.37987416582957	-29.85579573954440	5.84442854619791
C	33.77150613897810	-28.47729225463212	0.36403140126064
N	33.22502605833734	-25.54762288753479	4.88828909947467
N	34.68609470433893	-25.62021028686897	7.33280410088089
N	34.94457918023548	-27.53404750447374	3.80578506279112

C	32.92335259616369	-26.66357361631068	2.73082399331917
C	32.93566267040496	-24.00348245817211	6.76823658155674
C	36.41757302410107	-26.83504542508615	8.56492310477011
C	37.06077425444154	-28.70845803504582	4.15955146849492
C	30.63084643385179	-22.83699183273957	5.06267882850826
C	33.39751030947511	-22.95772910808769	9.64808785997287
C	38.87076465143925	-28.70476189215588	8.85095591066936
C	35.63198140591450	-29.73105936334905	1.27037639313543
C	32.56116079691200	-25.73720837203790	3.70518984000650
C	33.88088429213154	-24.55198193296683	7.62975882809903
C	36.90204318103108	-27.61060950897238	7.51563346183604
C	35.96510334725104	-28.34456992145165	3.38773419613779
C	31.47792757065884	-24.77676903500474	3.56827615484742
C	34.10555753184252	-24.10853044638463	8.99577903036104
C	38.08129176818826	-28.46060977970788	7.59898341068930
C	35.72060424947714	-28.81690303091954	2.03455369090180
C	31.51688550553455	-23.98818437032262	4.68829140991489
C	35.05139904397187	-24.94759489277982	9.52375133017360
C	38.29811956352667	-28.94108627242239	6.33589448125255
C	34.51561656686124	-28.29033015667691	1.65298745694354
C	32.60749879929239	-24.49171822841220	5.50682471905447
C	35.41238325938789	-25.87684746429681	8.46511332823760
C	37.23131816844483	-28.40660977969037	5.50433441498013
C	34.05531589983303	-27.47326647170721	2.76605399381055
N	36.40179946028243	-27.60756853243868	6.24187387690014
Fe	34.74676680289606	-26.66487351953088	5.60626388387984
C	32.89135349856146	-31.59245302195140	6.67067661997953
C	33.80185481067473	-32.15811665078174	7.75119019082687
C	32.33272136355582	-27.59539454731413	7.05963291201492
C	33.56305125278432	-27.96930693602286	6.28531518959979
C	33.77601719099307	-29.42918350202202	6.13747465331403
O	34.68741644793776	-29.98642906368462	5.56110457190168
C	32.78403720606617	-30.16112426303420	6.75663689508166
H	29.89151690236550	-22.62823122250574	4.28307956307470
H	31.20600771233806	-21.91533926116722	5.22365794677102
H	30.07793589850742	-23.03501939780263	5.99079845589742
H	31.07705626586111	-24.52952278767940	1.45592785706597
H	29.97768270672716	-25.64112534430982	2.27415030744508
H	29.81186978881847	-23.89933499780587	2.51528571033971
H	33.51815344502270	-27.51706483569939	-0.10451025207661
H	34.36184869598512	-29.04787246688403	-0.35978670577836
H	32.82769650607352	-29.01835581772236	0.51574799403938
H	36.27813236801312	-29.88610920988200	0.24621330162926
H	37.65250168575250	-29.33041664377660	1.20822495289834
H	36.70305855201575	-30.71865087134766	1.74530590103992
H	33.76326029887134	-22.78684191793492	10.66537711357784
H	32.31486631902527	-23.13091534502519	9.71457239429584
H	33.53844871893736	-22.02406421785778	9.08729825770244
H	36.73829027493791	-24.82353870941503	10.87100405375131
H	35.44959114885710	-25.89253780997214	11.42708756996155
H	39.71356174861161	-29.37871827280975	8.66884984648481
H	39.27986004682506	-27.77266415520912	9.26409953164995
H	38.25237831883143	-29.15840300800864	9.63706872011548
H	38.96726964488705	-30.80343223640368	5.47371595640192
H	39.94585446134685	-29.40533621835282	5.01807570382475
H	40.09493490199481	-30.09764402753144	6.63707209731085
H	35.24115906365047	-24.14060830543842	11.51533914259757
H	39.70604244254000	-22.77021475419307	4.25568203133431
H	38.57422896647671	-21.54049578897390	4.84625840280729
H	39.26157291677247	-22.72364083959993	5.96678922320056
H	33.46234718315555	-31.85143928228779	8.74433410522583
H	33.80161554275125	-33.25263496928663	7.71307442413959
H	34.82664280036910	-31.81108513155325	7.60928078828291
H	33.25277134358052	-31.86493506678028	5.67723074434656
H	31.86663199533059	-31.95088282967987	6.79021490022616
H	32.15655843762774	-26.52498992193243	7.07861513385956
H	31.44415894404922	-28.09173156490294	6.65150527766857
H	32.41301186128999	-27.94789624446154	8.09723382904116

H	37.22519908093835	-23.05517007177670	2.69451918529612
H	37.36301365764545	-24.72127086624823	6.54884911895514
H	35.38608905744385	-24.82135667409552	2.86108030070303
H	32.30771722145766	-26.71033006894912	1.83811649246121
H	36.91429942144185	-26.93429681305920	9.52482423498746
H	37.80008563861414	-29.35535946083111	3.69863316705036
H	32.36133807382860	-23.15980422066541	7.13727744931986

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B3LYP Scan/Melmid IPC Model/BSS/190 degrees Constrained Optimization

C	38.87281673439336	-22.57928687094996	4.87073311379355
C	37.72960984433931	-23.52060721039283	4.67541140486400
C	37.14509429517677	-24.44715072712408	5.50142969002287
N	37.00854213732747	-23.60668476404844	3.49237181502724
C	36.04579655885212	-24.55653480008353	3.64973723781263
N	36.10573025938128	-25.08010889169179	4.85404798111378
C	30.51650079463145	-24.79792002609054	2.46391514972654
C	35.73182698119364	-24.85718139265040	10.90580059237707
C	39.45407947203729	-29.79479072761212	5.87729141254088
C	33.77586735653720	-28.54345550908544	0.43568098172642
N	33.23260922257813	-25.57673490795245	4.93901286461041
N	34.72913679416909	-25.59374320586662	7.36291294320277
N	34.96648295505524	-27.55798042524891	3.86001014127754
C	32.92583537032910	-26.72014753332688	2.79547975483110
C	32.94587163516942	-24.01165602967810	6.80114954150465
C	36.49156693849136	-26.76814314872165	8.58939978303293
C	37.10078217023958	-28.70151018782705	4.20544987358046
C	30.60556658477967	-22.89831899565976	5.10683669245233
C	33.43606116363476	-22.91480978310859	9.65741820407681
C	38.96552123897444	-28.60869710847207	8.87333835998297
C	36.65495886744404	-29.76138646891573	1.33078038844889
C	32.56044711619556	-25.78858477597499	3.76399210375130
C	33.91287029408261	-24.53239810642743	7.65569986295480
C	36.97112368143434	-27.55334909904328	7.54531508451304
C	35.99172168245526	-28.36161737055352	3.44099175957981
C	31.46355812058403	-24.84407649741031	3.62671549428884
C	34.15046665244651	-24.06564916193698	9.01216454660392
C	38.16074536746720	-28.38891882156369	7.62668218008869
C	35.74010605166324	-28.85040689658660	2.09474323948467
C	31.50235091779401	-24.04282252233157	4.73789010487304
C	35.11520021139162	-24.88361846333852	9.53860738472848
C	38.36815092556122	-28.88476460857563	6.36823534177294
C	34.52696670870034	-28.33899819858166	1.71799269520640
C	32.60728176569886	-24.52225860384814	5.55133114870927
C	35.47388450282361	-25.82354106102352	8.48851574270879
C	37.28515277953446	-28.37496325913391	5.54221249687520
C	34.06744200503353	-27.51643961543166	2.82745772415457
N	36.45553565248699	-27.57392085316061	6.27796595023022
Fe	34.77954083898601	-26.66339071480653	5.65204761528838
C	32.73674368136174	-31.57096578503235	6.32793741667998
C	33.40836056397126	-32.24844588279193	7.51419880860625
C	32.37732805575581	-27.60904266678032	7.11802505400910
C	33.61004276903763	-27.97161033624389	6.34139925606909
C	33.79001213266844	-29.42771661585818	6.12574907569988
O	34.76957762898017	-29.99204566326934	5.68479809644856
O	32.67049994423337	-30.14433246947823	6.49382434828871
H	29.85946030667357	-22.70490645867602	4.32969285421099
H	31.17144451493715	-21.96896647476891	5.25589223410821
H	30.06024736877415	-23.09369784554509	6.04001847031168
H	31.04221992574161	-24.62306908467151	1.51535626019803
H	29.96403748061696	-25.74061256534451	2.35322387685631
H	29.77760337784510	-23.99883768160869	2.57875423363004
H	33.50302150861708	-27.58922529031321	-0.03407093258464
H	34.37025603728721	-29.10649919348507	-0.29079128764117
H	32.84237367848041	-29.09979267818431	0.59608313620072
H	36.29443069221580	-29.92871452182901	0.31084558919847
H	37.67059891882440	-29.35049006939986	1.25687678015840
H	36.74071606148971	-30.74428173820478	1.81302883466931

H	33.81080664725705	-22.72693822026343	10.66842352558218
H	32.35622931208530	-23.09936615975543	9.73771141633781
H	33.56035703972788	-21.98685969549098	9.08330979296471
H	36.81769015489337	-24.69860587152035	10.85921921846235
H	35.57045550528344	-25.80223522813623	11.44152108617535
H	39.81106273525877	-29.27939466914685	8.69192963590957
H	39.37215103994747	-27.66790679493451	9.26892341612949
H	38.35840946868707	-29.05544870987320	9.67208737680665
H	39.04677378124766	-30.74957603022945	5.51934760778513
H	40.00979425036234	-29.34771317859415	5.04208095008412
H	40.17737540947265	-30.02265758102881	6.66663031194759
H	35.31008413390862	-24.05679932853744	11.52160763411281
H	39.68610548832357	-22.76158178257467	4.15532860923673
H	38.56755975468823	-21.52931727877576	4.76557594784966
H	39.28425335486941	-22.70425374413306	5.87651487604324
H	32.89744810338404	-31.99479581467330	8.44706008782137
H	33.38139785762556	-33.33679658943095	7.39514737650105
H	34.45205273969079	-31.93940156053618	7.59152484772931
H	33.26633299908296	-31.79922917081091	5.40083829660006
H	31.69482020658360	-31.88432641632572	6.23302496961171
H	32.31216052419458	-26.54758297516728	7.33364562932216
H	31.47742834779466	-27.90325332381943	6.56178730285164
H	32.33038976932345	-28.16292319816234	8.06404058875526
H	37.16891895997279	-23.06161585288336	2.65748793828398
H	37.40385323931886	-24.69975080462939	6.51906014219117
H	35.33894727031559	-24.83097082974201	2.88053440624712
H	32.30252605962865	-26.78305166418059	1.90909796522969
H	37.00120755881147	-26.84815050092742	9.54429605111241
H	37.84209332372685	-29.34671552221535	3.74533830177795
H	32.36435465294711	-23.17129723078072	7.16655788360167

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B3LYP Scan/Melmid IPC Model/BSS/200 degrees Constrained Optimization

C	38.89148839421463	-22.60169371723730	4.75435477718832
C	37.72604301387025	-23.525268809719843	4.61480125319411
C	37.17919861880394	-24.45706400710831	5.46068756602657
N	36.93574464256599	-23.58481853471768	3.47519520303408
C	35.97210545683758	-24.52547195154025	3.67522813000831
N	36.09596958479867	-25.06800991625421	4.86618687224683
C	30.49587794862719	-24.88688477202234	2.52973339942742
C	35.80716404734613	-24.75106776003682	10.91552863599968
C	39.51550112295892	-29.74341679236581	5.93379590716966
C	33.77791309327277	-28.62092646043330	0.52276771299991
N	33.23886993071444	-25.60327533889069	4.99454979087340
N	34.76057470851585	-25.56701610161101	7.40272405842542
N	34.98953535737948	-27.57975290681815	3.92314749836229
C	32.93223526287903	-26.77437123147515	2.86495747289521
C	32.94534184435449	-24.02144186769143	6.84100178794956
C	36.55774577613099	-26.69296006939348	8.62307550718956
C	37.13549218144522	-28.70056301140222	4.26812311191700
C	30.57699018884281	-22.95915511614252	5.15186793564284
C	33.46002041731446	-22.86828110799691	9.67066981989060
C	39.04872210369813	-28.50710435701120	8.91266618671469
C	36.66986434073006	-29.81243086302376	1.41430002500419
C	32.56167528780474	-25.83686464710740	3.82619737379025
C	33.93100220515775	-24.51433222652355	7.69032215012972
C	37.03405175288390	-27.48949324293274	7.58644752783458
C	36.01630465822231	-28.38284516651291	3.50804615367584
C	31.45099364369611	-24.90906364059871	3.68680178671968
C	34.18123149418545	-24.02034034976466	9.03519194908370
C	38.23103200750985	-28.31406200893463	7.66998243274570
C	35.75595189550427	-28.89510790001106	2.17181811666293
C	31.48577868425820	-24.09637701118702	4.78995312218139
C	35.16762262392285	-24.81278791620433	9.56001126444630
C	38.42891778460624	-28.83100088296311	6.41870853152098
C	34.53729180976985	-28.39555152253257	1.79676021664257
C	32.60262069611802	-24.55202194289352	5.60067900837599
C	35.52524442286261	-25.76498228535701	8.52038694125016

C	37.33344808539008	-28.34418337020168	5.59517488182692
C	34.08157315437163	-27.55929031413816	2.89741355671829
N	36.50584761538226	-27.53531879801421	6.32485228395185
Fe	34.80948653154395	-26.65890778477284	5.70544025156298
C	32.66235899349651	-31.51133821053153	5.94242591669600
C	33.03193195862622	-32.32595817220697	7.17357005251579
C	32.42326603638659	-27.63761099249393	7.17759249712846
C	33.66270973060611	-27.97633398312339	6.39998869681793
C	33.82761735270464	-29.42437047408128	6.12127316952400
O	34.85016132106990	-30.00597172135770	5.82728714744624
O	32.63156135536584	-30.10116637460332	6.22495672044787
H	29.82492131437636	-22.78232712066199	4.37647695622172
H	31.13263092160577	-22.02178061112800	5.28877410805606
H	30.03848689605084	-23.15123689419574	6.08966773075368
H	31.01355723692106	-24.71988218826002	1.57537171444650
H	29.95109829913978	-25.83576557748454	2.43504257363589
H	29.75066084402886	-24.09289119820629	2.63902427104593
H	33.51320127619749	-27.67445323631294	0.03289583556283
H	34.36276866891574	-29.20644293735917	-0.19355836185991
H	32.83911088513668	-29.16305930741481	0.69960723974378
H	36.29741508699287	-30.00413089824620	0.40296865377660
H	37.68017196166718	-29.39309627176314	1.31812692973875
H	36.77234631130111	-30.78431558277706	1.91520686669199
H	33.84331754545082	-22.66092295359310	10.67463888239970
H	32.38327645628656	-23.06371307520774	9.76523111920480
H	33.56771417310809	-21.94776238781820	9.08137113265147
H	36.88689322417393	-24.56101949184223	10.84770159911056
H	35.68331638496009	-25.69377700457523	11.46507698835886
H	39.89617581687798	-29.17637359737048	8.73510175943583
H	39.45361795324116	-27.55736602376053	9.28822219194164
H	38.45126400796507	-28.94328546255613	9.72440056991121
H	39.10989087400979	-30.70582079457320	5.59489041046577
H	40.06249730533911	-29.30742452117146	5.08702868244630
H	40.24606840987912	-29.95506565099974	6.72098070837834
H	35.37254180742887	-23.95596672338537	11.52918520110187
H	39.65880667395928	-22.78547086530830	3.99014271275370
H	38.59542747796544	-21.54649280722552	4.68019417131830
H	39.35968583539005	-22.74547823264712	5.73245348256832
H	32.35046863341883	-32.11090558205463	8.00118261647247
H	32.97211049535093	-33.39679306005115	6.95190260924952
H	34.05113670450890	-32.10004921255675	7.49172578502080
H	33.36597719461909	-31.69641709638744	5.12860193593289
H	31.65095535053069	-31.74581676518278	5.60348319097243
H	32.40650133872552	-26.60461407796553	7.51227990653260
H	31.53590197216817	-27.80836934809759	6.55308287800141
H	32.30157529595906	-28.29372204272460	8.04819428425479
H	37.05410987220505	-23.02968158308462	2.63994575363042
H	37.49497946925201	-24.72895077399700	6.45704120520651
H	35.21811698231700	-24.78072360673085	2.94521256378576
H	32.30293449522584	-26.85464475789219	1.98422616511062
H	37.07994692831331	-26.75086706519959	9.57276214152331
H	37.87623105949828	-29.34998909205535	3.81305707737939
H	32.35492840779027	-23.18521569375646	7.20169705521083

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B3LYP Scan/Melmid IPC Model/BSS/210 degrees Constrained Optimization

C	38.87852649826284	-22.60012588302590	4.67608568154596
C	37.70883213075061	-23.52345646086207	4.57693172931046
C	37.20101990280660	-24.46747607216699	5.43373872741866
N	36.86853147784415	-23.56881753781612	3.47311802717228
C	35.91557729481237	-24.51337410815472	3.70313592912201
N	36.09275317368793	-25.07175280302162	4.88003044935097
C	30.47400709365584	-24.98355965611556	2.59378553347624
C	35.89412450570754	-24.64571036101649	10.90994054337579
C	39.56436802839166	-29.71980363071091	5.98818007898030
C	33.79025341407765	-28.68678808170562	0.59176482090044
N	33.24721294264601	-25.63481156364864	5.04309747716965
N	34.79041536581540	-25.55085937632411	7.43625384086920

N	35.00929298381323	-27.61323565106551	3.97993266175505
C	32.94296833286892	-26.82767630809233	2.92413943585510
C	32.94511452927348	-24.04057612717392	6.87713523826504
C	36.62400686533309	-26.62725123580300	8.64694016540113
C	37.15701854049470	-28.72813798487732	4.33029303711606
C	30.54177966762575	-23.03557891025129	5.20092894879225
C	33.49231884286885	-22.82572272879104	9.67490251574614
C	39.13333616478980	-28.41283763611770	8.94165697328104
C	36.68372949112336	-29.86976840010703	1.48820560842030
C	32.56549644514708	-25.88855084605191	3.88120634411666
C	33.95045697875663	-24.50502771628096	7.71899302290132
C	37.09197678679150	-27.44198427732031	7.62107400414951
C	36.03460443334041	-28.42065291345784	3.57025031491898
C	31.43854570631382	-24.98048469090453	3.74331321059947
C	34.21796049508282	-23.98044605714644	9.04932523839295
C	38.29547521141846	-28.25663635948298	7.70717452147252
C	35.77053234958620	-28.94701801012511	2.24012430098789
C	31.46724403120785	-24.15974865161301	4.84071319876898
C	35.22691888083706	-24.74632991386067	9.57009108572812
C	38.47787954744297	-28.80380965462920	6.46662662956094
C	34.55135190278368	-28.45021858212647	1.86277005744830
C	32.59798892925013	-24.59002907750442	5.64614468001750
C	35.57835407446724	-25.71450388591590	8.54280956244224
C	37.36817207790690	-28.34249459275044	5.64708795686737
C	34.09769940391536	-27.60439662666602	2.95687826309756
N	36.54666634899857	-27.51977523044650	6.36814888562247
Fe	34.83519983208975	-26.66618698220963	5.75332756153724
C	32.6091181135338	-31.41025254033173	5.60079655386600
C	32.67938154479085	-32.32307298623773	6.81561979893351
C	32.47063188533382	-27.65951188360938	7.24941562627772
C	33.70489006635091	-27.98061278568658	6.45554238568301
C	33.84415803018225	-29.42170626429962	6.12199934261191
O	34.87100681834976	-30.04467557264067	5.96650301317867
O	32.61357466432727	-30.02189832363297	5.98028719103879
H	29.78262775962016	-22.87588630064142	4.42869293323182
H	31.08271219320142	-22.08841964592570	5.32912075210462
H	30.01174791579134	-23.23067054016895	6.14292941999448
H	30.98205584033356	-24.82383430382981	1.63306261531124
H	29.93860901474519	-25.93929897168259	2.51605495684266
H	29.72144054511673	-24.19594748439366	2.69882470148439
H	33.51119654238605	-27.74428019999689	0.10246005949659
H	34.38041806324380	-29.26475362059665	-0.12639587331607
H	32.85940210427275	-29.24156139251956	0.77193730584919
H	36.31171866234936	-30.06631792108774	0.47764009563289
H	37.69450361864612	-29.45201740015635	1.39055721928383
H	36.78516147401262	-30.83933597919311	1.99389185656805
H	33.89224158980146	-22.59208037224278	10.66656290251848
H	32.42059688196756	-23.03438503729945	9.79497176864610
H	33.57503539840538	-21.91636984889304	9.06464353245804
H	36.96927199539658	-24.44195274262748	10.81473694128121
H	35.79584112959907	-25.57753193891044	11.48276347973717
H	39.98336402004605	-29.07959611275138	8.76711201500465
H	39.53617787069307	-27.45110589684669	9.28783362258695
H	38.55191144281989	-28.83384604578380	9.77275073026949
H	39.16041306490792	-30.68952504511305	5.66892082258102
H	40.10279407355201	-29.29578057103689	5.12982931417575
H	40.30224063816840	-29.91505995378665	6.77283379328421
H	35.46092382723749	-23.84339806241116	11.51514966024671
H	39.61649084513510	-22.78033667493125	3.88261762754987
H	38.57942902664183	-21.54482759769002	4.61761059499575
H	39.38352112011537	-22.74778526680001	5.63511335617776
H	31.87119181536870	-32.09904302056711	7.51710730166642
H	32.58644869361517	-33.3705230952566	6.50990563617095
H	33.63363670607644	-32.20172321641117	7.33175691054756
H	33.44519781980695	-31.59690141924570	4.92439953503733
H	31.67075731379630	-31.54419012760581	5.05832743953515
H	32.46733891032883	-26.64063906931611	7.62651804604365
H	31.58324752854992	-27.79391749825759	6.61691004063433

H	32.34194411513120	-28.34784644818306	8.09463316931972
H	36.94934864354617	-23.00265303581248	2.64080343523399
H	37.56142840194995	-24.75304977212425	6.41093084977170
H	35.13002549580806	-24.75983455207815	3.00411417950850
H	32.30937039725308	-26.92107977394216	2.04780328771361
H	37.16184900044115	-26.65911764381082	9.58910760779445
H	37.89495747741601	-29.38534576420956	3.88190730476992
H	32.34576250503050	-23.20919257281497	7.23439257871227

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B3LYP Scan/Melmid IPC Model/BSS/220 degrees Constrained Optimization

C	38.86875694630750	-22.60210341496395	4.68062468426822
C	37.70482799186600	-23.53206747991890	4.57548267731430
C	37.18465542798262	-24.46268633176009	5.43936146664321
N	36.88559857532412	-23.60051780172626	3.45707675767534
C	35.93186552717118	-24.54456163739968	3.68618413096748
N	36.08901518330715	-25.08107882306548	4.87606892567052
C	30.47227165532846	-24.98695713362999	2.58511483717832
C	35.88733502258948	-24.62845336669790	10.90579086833047
C	39.54609760565346	-29.73623033745811	6.00466254837538
C	33.78270315732703	-28.70207960485354	0.59698827565408
N	33.24343304796304	-25.63551296619044	5.03730552473183
N	34.78411457830442	-25.54475862784492	7.43439477494814
N	34.99782883256475	-27.62437421471994	3.98552671776697
C	32.93846870215619	-26.83252253607646	2.92121125359866
C	32.93686519635968	-24.04022107155324	6.87168077253349
C	36.61955976018064	-26.61588495679600	8.64760510361925
C	37.14341152946685	-28.74205363036443	4.34150619571083
C	30.53426283255558	-23.03918420265934	5.19206634018573
C	33.47954409455733	-22.81828856007122	9.66732314212384
C	39.12274499431183	-28.41016912770802	8.95067210477632
C	36.67038099217670	-29.89332456723118	1.50281795172563
C	32.56257295012060	-25.89016898150701	3.87526005654302
C	33.94283820324917	-24.50007078432033	7.71475276555946
C	37.08748734340305	-27.43449971288631	7.62451864721780
C	36.0218477174939	-28.43589527057800	3.57974880435527
C	31.43565456490547	-24.98251891776075	3.73557731005128
C	34.20859660298557	-23.97203804345166	9.04402387992019
C	38.28660622572696	-28.25481669298462	7.71491316203094
C	35.75828614104205	-28.96621257239391	2.25082285635761
C	31.46159482463474	-24.16225700561353	4.83315492716139
C	35.21962160863932	-24.73398051091419	9.56651735329533
C	38.46564576505427	-28.81026885456028	6.47749893511116
C	34.54171437807223	-28.46616737076274	1.86943395379890
C	32.59197797712034	-24.59163786091529	5.64020669641413
C	35.57294952432159	-25.70398538982607	8.54119511750618
C	37.35845424188577	-28.34748003339357	5.65535034329057
C	34.08907048783669	-27.61499120654499	2.95999124109835
N	36.54268722969488	-27.51538416643530	6.37152147086167
Fe	34.82980217814951	-26.66459963132885	5.75365174264364
C	32.59718648640973	-31.34660590798181	5.47749739526758
C	32.64164735370768	-32.32381712695840	6.64272596316900
C	32.60820726812565	-27.65097768566026	7.44769138942041
C	33.72600090370956	-27.97204177434560	6.49645360015108
C	33.84228599458167	-29.40988350973253	6.13876439645815
O	34.86292502112197	-30.04855620177992	6.01003910266473
O	32.60854584954573	-29.97803797002685	5.92574300782854
H	29.77626191101004	-22.88034495726226	4.41852735513930
H	31.07388615604588	-22.09139115127550	5.32117358292190
H	30.00276817956791	-23.23483532529066	6.13312681662671
H	30.98154174826412	-24.82956485159282	1.62466300868915
H	29.93621791909823	-25.94243611626569	2.50892892164567
H	29.72028466785831	-24.19848042064067	2.68777935047181
H	33.51446394951297	-27.75940412706337	0.10190822434741
H	34.36962963798739	-29.28938178537689	-0.11624068243266
H	32.84578953373054	-29.24663062582920	0.77672579305686
H	36.29740009213236	-30.09462459199144	0.49353674623393
H	37.68129611805821	-29.47660241987761	1.40214773213896

H	36.77189460503417	-30.86043175313066	2.01313566383536
H	33.87512879969447	-22.58476698619241	10.66076463823838
H	32.40754034233167	-23.02812081164531	9.78291513151363
H	33.56368011058360	-21.90845130501129	9.05796710097226
H	36.96042576773830	-24.41421188043531	10.80985157727495
H	35.79877652924672	-25.56173301568582	11.47783512967640
H	39.97125676063927	-29.07948611080944	8.77865707643130
H	39.52753815834537	-27.44865072914871	9.29509892579917
H	38.53938860479269	-28.82794221596819	9.78209750266023
H	39.13582408657305	-30.70560860847183	5.69242763175269
H	40.08647543700192	-29.32154935820587	5.14299749474288
H	40.28333539506505	-29.93068158868357	6.79011312219658
H	35.44708088280832	-23.83103151967698	11.51236971725185
H	39.61990073533394	-22.78943243035233	3.90133222310161
H	38.56613471287547	-21.54898959632560	4.60348661443709
H	39.35913227144366	-22.73482468215173	5.64937461345044
H	31.82429585484958	-32.13194005543681	7.34327177585808
H	32.54480033873937	-33.35207044790941	6.27848764368496
H	33.58887211313548	-32.23860548418130	7.17787791095081
H	33.44115575326225	-31.50664761452281	4.80380889135666
H	31.66603297127886	-31.44221978056396	4.91512645484187
H	32.23522225466650	-26.63626187999455	7.32152462380558
H	31.77691155382120	-28.35386863868127	7.35705724267277
H	32.98218857577774	-27.71759932284638	8.48104061253137
H	36.97949723304082	-23.04861612803758	2.61661717905546
H	37.52782266761545	-24.72933454082070	6.42798178469324
H	35.15975662276887	-24.80585568134586	2.97764442932495
H	32.30648942205536	-26.92578620517014	2.04371378970160
H	37.15718523883229	-26.64517050969763	9.59002333366500
H	37.87845020874877	-29.40529317294685	3.89721525043021
H	32.33513451438577	-23.20953409113170	7.22665259327926

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B3LYP Scan/Melmid IPC Model/BSS/230 degrees Constrained Optimization

C	38.89817057762306	-22.67300585177511	4.57112377195124
C	37.70454635714936	-23.56916447052636	4.52031993057641
C	37.20202405008533	-24.48966506395590	5.40522878146132
N	36.83118257735407	-23.61115406365620	3.44238816827751
C	35.86530087719292	-24.53131066611868	3.71369028691902
N	36.06528561156220	-25.07731716788964	4.89277888779727
C	30.44177599954768	-25.01908900431401	2.65771653463917
C	35.96731633537627	-24.51599495016188	10.90402171563779
C	39.52152156868219	-29.76642425482836	6.07521100738103
C	33.72288875260730	-28.76636939086366	0.69487421518599
N	33.22700722209588	-25.64113793049830	5.10212224968580
N	34.80022531673022	-25.50897048324963	7.47500776468345
N	34.98025767453540	-27.64375912290238	4.05292301546688
C	32.91187235067590	-26.85963802209915	2.99871910259004
C	32.92993576538547	-24.02861691861864	6.92068864027434
C	36.66651717973194	-26.54356033132043	8.67248670128019
C	37.11551307866024	-28.77924778141782	4.41366973546431
C	30.51379135157822	-23.04876509515604	5.24714268992457
C	33.51267249408470	-22.75564092125655	9.68544049506812
C	39.15477883850320	-28.35517573397031	8.98857827954045
C	36.60618610422868	-29.97418459725725	1.59596126086507
C	32.54026619732675	-25.90843591713650	3.94610347284896
C	33.95260770003072	-24.46890721967688	7.75440867691159
C	37.11683537995404	-27.38606849495983	7.66141035648809
C	35.99205266948503	-28.47373155533475	3.65305216338815
C	31.41014080508033	-25.00431622640566	3.80402624744619
C	34.23992466023432	-23.91425888910074	9.06892517942230
C	38.30778402158566	-28.21798327628160	7.75815674804192
C	35.70983904645728	-29.02579380111989	2.33679517296674
C	31.43979762451079	-24.17492593939996	4.89451043525473
C	35.27076122182505	-24.65486909113646	9.58263260319700
C	38.46311020163539	-28.80902784730899	6.53470440085418
C	34.49529521498445	-28.51806115116801	1.95705261561632
C	32.57624141024493	-24.59419723125474	5.69861685799173

C	35.61273164839097	-25.64008241845839	8.56772639445877
C	37.35192825303394	-28.35198563258897	5.71395782970350
C	34.06090049122189	-27.64434827153569	3.03631243896523
N	36.55596229905824	-27.49057969516021	6.41741225442434
Fe	34.83183743677383	-26.65191673261110	5.81149626567483
C	32.86378453476641	-31.27585270330782	5.17202420817530
C	32.59604579039406	-32.28390939984713	6.27887070720187
C	32.50606945431058	-27.69434554236015	7.34732303640234
C	33.74482315890997	-27.95817480863992	6.54099288863339
C	33.92491924753484	-29.39659485229167	6.20275247058782
O	34.92399492428368	-30.05988179671681	6.35990256174668
C	32.78462882832901	-29.91700652497222	5.64983748886819
H	29.74884013414094	-22.90070347043930	4.47827886547031
H	31.05322463141772	-22.09868099558165	5.35941039443931
H	29.99083134745975	-23.23280212913581	6.19529399057023
H	30.94669445247015	-24.86996088478602	1.69364101414007
H	29.90517796703301	-25.97506715303271	2.59178883702745
H	29.69030861322068	-24.22961705522735	2.75677892768419
H	33.49272071595234	-27.83112580633480	0.16719756956611
H	34.28227757666647	-29.40229289860815	0.00160022546259
H	32.76438418979421	-29.26374092131463	0.89539650170775
H	36.21272668776376	-30.20218857598748	0.60023112593634
H	37.61509844258352	-29.56150761610025	1.46328830864373
H	36.71852419582703	-30.92749488960729	2.12950014235220
H	33.92170117178481	-22.50448604707313	10.66908924192625
H	32.44384053425406	-22.96991260910951	9.82026936595475
H	33.58215738867304	-21.85473271063485	9.06105319469191
H	37.03324118457750	-24.28148609063112	10.77955850364122
H	35.91136691045342	-25.44215573058538	11.49147311186059
H	39.99747081301690	-29.03289657760021	8.82103446487542
H	39.56860716030977	-27.39004519738653	9.31148302330046
H	38.57660038235304	-28.75417881948281	9.83273863950794
H	39.09008618651899	-30.73667106050048	5.79581042015862
H	40.05883351868699	-29.38636629275837	5.19583205350657
H	40.26459499408822	-29.95208909499791	6.85729843871774
H	35.52497195376246	-23.71861450879916	11.50915411841697
H	39.60887372694791	-22.88468980536554	3.76072137570936
H	38.62340117097582	-21.61171107480543	4.50309195085189
H	39.42627431895171	-22.81779474954691	5.51807854527661
H	31.62340427858181	-32.10343912966217	6.74470003122928
H	32.59586309792046	-33.30044833602393	5.87142207278691
H	33.36930139794070	-32.22441668460974	7.04628356120452
H	33.84792825526872	-31.43509244192458	4.72810203081524
H	32.10460744177964	-31.33221075015472	4.38943810767720
H	32.43858721543944	-26.66653918489478	7.69490224912311
H	31.62198487394059	-27.91195282307897	6.73365641052088
H	32.44319054381760	-28.36196618970117	8.21828889315681
H	36.90004307877528	-23.05904894553410	2.59967466795640
H	37.58470419907233	-24.77042240337141	6.37518766990029
H	35.05487389610005	-24.77054967175180	3.04113498811457
H	32.27264858692435	-26.96267564578152	2.12750710174667
H	37.21927743352241	-26.55244745190314	9.60653772228923
H	37.83724721153030	-29.46298362652713	3.97866941394677
H	32.32727280094914	-23.19768320203785	7.27356971819536

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B3LYP Scan/Melmid IPC Model/BSS/240 degrees Constrained Optimization

C	38.89090856305620	-22.67085159845504	4.56196924351807
C	37.69951296321459	-23.57013490851290	4.51421547179314
C	37.20159749177959	-24.49172005495056	5.40056392054967
N	36.82308878914907	-23.61395742720198	3.43886799226424
C	35.85977433631799	-24.53596515156894	3.71307653472505
N	36.06434291160217	-25.08155217480924	4.89162085941674
C	30.43322457218628	-25.02289628449455	2.67072545462336
C	35.99395393585323	-24.48664319159246	10.89386650738632
C	39.49683931952261	-29.80208599138433	6.09608772288284
C	33.70594140183384	-28.77627386807004	0.70870620010425
N	33.22558657532375	-25.63765377582488	5.10885413510688

N 34.80568858708438	-25.49899557073854	7.47752242565213
N 34.97270999233582	-27.65017394225547	4.06209041537899
C 32.90865671961964	-26.85674495153072	3.00620595919901
C 32.92772297007156	-24.02685868991620	6.92900006201956
C 36.68128760954976	-26.52484820835044	8.66843848351685
C 37.09386014354736	-28.80990655280862	4.43191801672256
C 30.50181278562797	-23.05692799086236	5.26373930496554
C 33.52123498207558	-22.74371647003940	9.68733231556614
C 39.16048926012594	-28.34724280310042	8.99113201989701
C 36.57401755073182	-30.01285608768090	1.61911206541258
C 32.53772528645637	-25.90572510839840	3.95373490931738
C 33.95631649432170	-24.46127224951037	7.75867594936032
C 37.12319257318572	-27.37804983085626	7.66263996791734
C 35.97473876378621	-28.49521598687500	3.66817710880878
C 31.40428871002309	-25.00503254945075	3.81466161966159
C 34.24977749133126	-23.90084591775999	9.06963443517542
C 38.30785959068122	-28.21842676659776	7.76367154505509
C 35.68727895301598	-29.05128822921631	2.35467324739980
C 31.43238677583155	-24.17782786760493	4.90657915788522
C 35.28764600169791	-24.63461788979766	9.57863498599994
C 38.45054505641566	-28.82790698842426	6.54791476823995
C 34.47951294009938	-28.53061180866198	1.97076977977716
C 32.57247429138310	-24.59384589846108	5.70781500783642
C 35.62607222422391	-25.62286104054903	8.56519588169627
C 37.33958424432911	-28.37063625700225	5.72673725228346
C 34.05369675666408	-27.64722492619078	3.04553383717726
N 36.55553851657898	-27.49221123905185	6.42247515582689
Fe 34.83241228445889	-26.64784689057358	5.81613106061899
C 32.98282478224401	-31.24622643166159	5.07945429544671
C 32.53295495913159	-32.23746258041224	6.14139073508596
C 32.53548030386565	-27.70100897865968	7.39127549247978
C 33.75598146608849	-27.94617771118909	6.55346280055909
C 33.94834853254687	-29.38857630586192	6.23397115969962
O 34.90369476891495	-30.06919507221614	6.52746966819818
O 32.87928155922140	-29.88181448491425	5.54006491019180
H 29.73417713581158	-22.91115963400294	4.49711359999784
H 31.03678361619530	-22.10439475243605	5.37665498439097
H 29.98219981646981	-23.24552569421614	6.21285240555489
H 30.93560048782350	-24.87464699567590	1.70520064974477
H 29.89791487929225	-25.97981528661199	2.60762534344225
H 29.68082987526198	-24.23437370952994	2.77035246898245
H 33.49067493391821	-27.84152367395539	0.17387419803641
H 34.25722144563110	-29.42529260437699	0.02110438603103
H 32.73968297725661	-29.25778901085259	0.91067421023565
H 36.17758980530614	-30.24339258225624	0.62514868653388
H 37.58660290036910	-29.61040338659010	1.48293592715784
H 36.67842581476170	-30.96406150273508	2.15810148756736
H 33.92829420307609	-22.49472193345451	10.67235878034403
H 32.45225259198602	-22.95871617160053	9.81962997322084
H 33.59150782791034	-21.84118764239781	9.06529717268705
H 37.05389387607392	-24.23058261030183	10.76026957223437
H 35.96199589651687	-25.41566405210362	11.47847822873761
H 39.99937655471827	-29.03023476879474	8.82590236521526
H 39.58016742818714	-27.38082759047623	9.30242739922710
H 38.58505112783889	-28.73561814329579	9.84209520491377
H 39.05477579398483	-30.77322062941368	5.83691236445580
H 40.03026536343886	-29.44197521981043	5.20603458256329
H 40.24471681605782	-29.98096134740215	6.87519024604267
H 35.54188042347891	-23.70018599036604	11.50608047532683
H 39.59971730386560	-22.87992373249859	3.74924079732587
H 38.61299104654364	-21.61025983473863	4.49563005829757
H 39.42227244741075	-22.81489145343805	5.50721185125752
H 31.51543558632653	-32.01694063205804	6.47535934080605
H 32.54609605446857	-33.25522382773957	5.73728770722357
H 33.20035234119724	-32.20446968846550	7.00410624388037
H 34.01364253544595	-31.43796676893515	4.77715710986091
H 32.33816145358908	-31.28410575954895	4.19944575186035
H 32.40254726259572	-26.65496395369675	7.65462052491333

H	31.64365583510223	-28.04367099598081	6.85003842499249
H	32.57439682240695	-28.28914915660288	8.32023222190792
H	36.88821992411194	-23.06163802336043	2.59601682835887
H	37.58751981117994	-24.77151802033549	6.36948642128102
H	35.04765573755233	-24.77651836012275	3.04307883846666
H	32.26879833589345	-26.95926387310277	2.13538010444945
H	37.23966049939437	-26.52747739102513	9.59921393161564
H	37.80672170935275	-29.50632358969676	4.00234997970677
H	32.32322590009088	-23.19784139495185	7.28330300875229

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B3LYP Scan/Melmid IPC Model/BSS/250 degrees Constrained Optimization

C	38.88014032392372	-22.65393119205988	4.55525577581231
C	37.69370566519189	-23.55951923739969	4.50367071861987
C	37.19845369062396	-24.48420599572609	5.38821573302227
N	36.81906412592681	-23.60574966604163	3.42697849937314
C	35.85926904556518	-24.53218019233466	3.69862460670078
N	36.06436448814415	-25.07823369914190	4.87689186235662
C	30.42515051193363	-24.98680133178076	2.68318229904752
C	36.02803151546906	-24.49609159113234	10.88183873053414
C	39.46592462481345	-29.84496283361877	6.06897279634470
C	33.65753706999942	-28.76483996389857	0.70700669609642
N	33.22401345651120	-25.62174955706133	5.10905381297384
N	34.82082566768820	-25.49128720241258	7.46708629692568
N	34.95640662928357	-27.64233263056478	4.04934401685729
C	32.89482804582669	-26.83040128600804	3.00261453985564
C	32.93461935447146	-24.02170340297288	6.93968923315162
C	36.70628388888802	-26.51999849356130	8.64120530512240
C	37.05776526393865	-28.83923142606520	4.41824704759461
C	30.50269635120261	-23.03967899507615	5.29081579313687
C	33.53802054035062	-22.75824851360537	9.70488689372303
C	39.17490461203081	-28.35826660501595	8.95266388401495
C	36.50670695548969	-30.04614837822038	1.61296037822426
C	32.53200620760988	-25.88100146213823	3.95461015146049
C	33.96910695127583	-24.45927177037714	7.76066081681987
C	37.13576064776122	-27.37869942093613	7.63477099642792
C	35.94067170951612	-28.50892174903868	3.65728795896698
C	31.39950499695906	-24.97733665065202	3.82437041198423
C	34.26899793659965	-23.90631436056447	9.07336573233191
C	38.31280687822839	-28.23022756742210	7.73184550173039
C	35.63879352803512	-29.06698293593685	2.34781835644494
C	31.43162815657778	-24.15807638100853	4.92187501242906
C	35.31438366032989	-24.63785877009195	9.56991404832140
C	38.43600166472655	-28.85371273941185	6.52123856927084
C	34.43932613147236	-28.52669487263648	1.96548383182179
C	32.57442285718514	-24.58053310202686	5.71631931602127
C	35.64972657807174	-25.61851532792836	8.54819150562979
C	37.32246159482867	-28.39070387995467	5.70647118889131
C	34.03245606207948	-27.63163331390424	3.03793473419537
N	36.55574406416272	-27.49613614606968	6.40084001848730
Fe	34.83383057920805	-26.63763665020882	5.80388887999766
C	33.20054352870234	-31.30448869465397	5.14796558331520
C	32.44564746509258	-32.18787500099400	6.12868165126350
C	32.53447789880654	-27.69528683038090	7.37053308080112
C	33.77125235973084	-27.93145355746584	6.55431417560121
C	34.01034464397596	-29.38352985265156	6.32151742991555
O	34.90106017653438	-30.04142453640499	6.80672994735330
O	33.06655961739891	-29.90745773756772	5.48838967154102
H	29.72885350928174	-22.89184533211546	4.53088060768711
H	31.03736664898722	-22.08691813703002	5.40337592427198
H	29.99091193525717	-23.23285683096693	6.24324053439595
H	30.92403971230722	-24.82613759991257	1.71779668487499
H	29.89354468082062	-25.94516915451157	2.61123526103353
H	29.66979978649450	-24.20251572159776	2.79336403163740
H	33.45534126805428	-27.82883304724725	0.16923353014652
H	34.19629860274637	-29.42499671887947	0.02009044605480
H	32.68438330989432	-29.23002993543163	0.91392355265506
H	36.10174459824114	-30.27551940632077	0.62214563652248

H	37.52474921115709	-29.66024388402715	1.46950793257656
H	36.59930209650680	-30.99637270794294	2.15585251900581
H	33.94935645298966	-22.51551622210613	10.68970435926439
H	32.47095742568650	-22.98009605828418	9.84139681559910
H	33.59993764475861	-21.85003672432780	9.09028952107702
H	37.08568902364630	-24.23294183532622	10.74393423695900
H	36.00483800909423	-25.42990846460440	11.45914743970730
H	40.00984445015514	-29.04503762027538	8.78304088036869
H	39.60076894183404	-27.39250136240123	9.25735544346247
H	38.60465319359660	-28.74184104164414	9.80927350780218
H	39.01006150133446	-30.81377511965847	5.82515948349920
H	39.99437968018160	-29.50115798232679	5.16954760496225
H	40.21962523856894	-30.02430000542024	6.84231139073820
H	35.57520289704865	-23.71714085135857	11.50303253448196
H	39.59097831265271	-22.85640893586324	3.74264147144677
H	38.59627857800320	-21.59471712373226	4.49194590623111
H	39.41126369763111	-22.79784010877830	5.50065494325271
H	31.39481345796372	-31.89256571007676	6.19094981597770
H	32.48698916445094	-33.23375235568417	5.80693061855027
H	32.88635151549703	-32.12172362190731	7.12546288971958
H	34.26046101286678	-31.56099512326226	5.12441020831849
H	32.78910787578777	-31.38189618942046	4.14006268854957
H	32.37579971594765	-26.64728884797013	7.61114474895019
H	31.65773126897925	-28.06448319841434	6.82055228173806
H	32.57161593956316	-28.26662151119177	8.30979108612120
H	36.88282204483118	-23.05188982183899	2.58504916555361
H	37.58400816905538	-24.76319126894527	6.35748028503466
H	35.04876925663622	-24.77493695251600	3.02746802711631
H	32.25099308818038	-26.92713160682876	2.13401863172007
H	37.27210071751815	-26.52314393920908	9.56746819823279
H	37.75620486015104	-29.55046106718854	3.98908234253692
H	32.33065076849794	-23.19626144233132	7.30308702165440

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B3LYP Scan/Melmid IPC Model/BSS/260 degrees Constrained Optimization

C	38.86439068829111	-22.64725108673614	4.57057073711021
C	37.68462402830230	-23.56115738419032	4.51243810000483
C	37.18789642031403	-24.48596551800010	5.39609526901127
N	36.81870711004997	-23.61601004500256	3.42914748041766
C	35.86185462759433	-24.54665170281499	3.69659402179969
N	36.06073018785744	-25.08773557438008	4.87829146577630
C	30.42487125547751	-24.96381102699814	2.67902047464452
C	36.04239344630088	-24.48566795161930	10.87072836724868
C	39.43868606453548	-29.87342967548722	6.07301168473985
C	33.63988200477946	-28.75613601173520	0.70329165585762
N	33.21741212989515	-25.61576502299121	5.10779843484549
N	34.81551207627071	-25.49179279250096	7.46591735751758
N	34.94183348102719	-27.64284365549680	4.04749201009929
C	32.88775502658657	-26.81668274701950	2.99738752521031
C	32.93252616107668	-24.01739931753436	6.94062610938509
C	36.70375438289454	-26.52092846894987	8.63581651567229
C	37.02691333493124	-28.86615727664625	4.42496605442684
C	30.50365346348757	-23.02568920407412	5.29354786047497
C	33.54804428121181	-22.74921179282356	9.70089602780996
C	39.16931862502769	-28.36280170620820	8.94631627243475
C	36.47406992043264	-30.06471701434112	1.61728030653505
C	32.52673802184561	-25.86865184892926	3.95132317694098
C	33.96759304361039	-24.45700594928376	7.75997782861669
C	37.12472221607397	-27.38817866609205	7.63324976834902
C	35.91640394655199	-28.52194365942997	3.66009082754355
C	31.39725745104141	-24.96081301503305	3.82188467512081
C	34.27421867841302	-23.90052596107940	9.06970401087607
C	38.29926282422336	-28.24311115478726	7.73029182600396
C	35.61290040170539	-29.07793894730532	2.34997117567954
C	31.43000705916430	-24.14536164004996	4.92201994534817
C	35.32105627958537	-24.63182049804746	9.56345317520890
C	38.41294986588956	-28.87729749164094	6.52423239909155
C	34.42071464409045	-28.52501346595039	1.96362095539324

C	32.57069175470735	-24.57364562162522	5.71670884209283
C	35.64923007603782	-25.61700755347252	8.54364745117538
C	37.29731613215660	-28.41534319894346	5.71159889402097
C	34.02035273665162	-27.62486994973716	3.03446525429280
N	36.53743751503431	-27.51267814703877	6.40325920840504
Fe	34.82165470209198	-26.64047136015818	5.80259698132954
C	33.35226418349684	-31.32574101182811	5.14838446710953
C	32.49036415882463	-32.17697174082841	6.06734121344333
C	32.52063528618311	-27.68491021875650	7.37373032379795
C	33.75551951839351	-27.92602093498582	6.55630589531218
C	34.00503257396453	-29.38482724203346	6.37906321805836
O	34.79841743491892	-30.03854152140646	7.01623421531203
O	33.19215401851565	-29.91691725065573	5.42750677970721
H	29.72943417784483	-22.87512575166971	4.53454864743434
H	31.04023988492531	-22.07412809802607	5.40720914773178
H	29.99237955261177	-23.21945903803935	6.24611890306996
H	30.92545535593295	-24.79812675503968	1.71534191114302
H	29.89308461751857	-25.92160726552166	2.60096165740436
H	29.66956145925398	-24.17990039976022	2.79210108261270
H	33.44790368385819	-27.81857913084861	0.16445726817804
H	34.17394079485636	-29.42178898135693	0.01800207480481
H	32.66188631606597	-29.21186965823088	0.90835833275684
H	36.06810474338968	-30.29266486168234	0.62655382095913
H	37.49496054475057	-29.68628927632952	1.47376708010222
H	36.55981188596154	-31.01488741138272	2.16138071269759
H	33.96476691983118	-22.50361012580438	10.68273706946777
H	32.48140424140600	-22.96918540029139	9.84362556154964
H	33.60798718887518	-21.84322962994475	9.08282755900547
H	37.09916397923396	-24.22273445222829	10.72561394104613
H	36.02290260530341	-25.41743471691075	11.45142904863871
H	40.00227035767080	-29.05196079582575	8.77657281676571
H	39.59853194275234	-27.39518114799503	9.24021696904810
H	38.60435972603324	-28.73870906696999	9.80974604898588
H	38.98027229302695	-30.84256887563009	5.83517268016283
H	39.96488417799602	-29.53508057362548	5.17017898471859
H	40.19464380854755	-30.05085167677956	6.84456574101428
H	35.59315500633257	-23.70459337156190	11.49188018712116
H	39.58225553345255	-22.84599682506535	3.76323306129176
H	38.57341986729141	-21.59018464149468	4.50332495884836
H	39.38995591844466	-22.78553564041686	5.51989940683448
H	31.4414977752223	-31.87381840420348	6.00979877469076
H	32.55626684488526	-33.23155418230048	5.77998971466402
H	32.82433107679739	-32.08533087419450	7.10256396985536
H	34.40730630610575	-31.58576254124982	5.24599980714582
H	33.05226823155029	-31.43043524723638	4.10449551239367
H	32.35379534979698	-26.63426797229832	7.59657624165450
H	31.64310870030495	-28.06992143150220	6.83452765112261
H	32.56946043801890	-28.24088756932357	8.32131357296807
H	36.88533303256250	-23.06399801736088	2.58622980420080
H	37.56737015862461	-24.75896759142541	6.36945556861870
H	35.05742924530577	-24.79528746764195	3.02034546894347
H	32.24541022155773	-26.90838630137436	2.12712926192646
H	37.27437663494116	-26.52030942817091	9.55912926500305
H	37.71897361721467	-29.58453190226066	3.99724757538062
H	32.33142952712677	-23.19018056937636	7.30474059878642

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B3LYP Scan/Melmid IPC Model/BSS/270 degrees Constrained Optimization

C	38.87476444717740	-22.66826685599371	4.57292135525014
C	37.68599629224158	-23.57027459473300	4.51285806000109
C	37.18226244494864	-24.49437136457941	5.39324953784343
N	36.81782278085123	-23.61230531693151	3.43079911388751
C	35.85323905918462	-24.53573345369339	3.69547482324557
N	36.04921888507899	-25.08396591460171	4.87433933017814
C	30.41928985684602	-24.91673243435284	2.66575164394457
C	36.03295000690014	-24.49323594441860	10.86344642756565
C	39.37988128386017	-29.91829191358690	6.07192112776255
C	33.60288161505298	-28.73765606016751	0.69278032378936

N	33.20138492755297	-25.59755500174323	5.09868826982491
N	34.79973210269829	-25.48670709775636	7.45711055574117
N	34.91746645183202	-27.62732351681267	4.03301500069924
C	32.86758756029614	-26.78924749927000	2.98427153342779
C	32.92660932444574	-23.99961812020613	6.93370090533603
C	36.67966561514793	-26.53161610920712	8.62702029713561
C	36.98772561772017	-28.87511755583957	4.41417298543771
C	30.50782359612650	-22.98606439377642	5.28563179875492
C	33.55145351656635	-22.73736179809213	9.69429297688250
C	39.11915772035181	-28.40647132754669	8.94539767193157
C	36.42735679657317	-30.06720235313366	1.60695628540030
C	32.51117172108621	-25.84161168144142	3.94034872513562
C	33.95911540627811	-24.44656349111812	7.75233075405849
C	37.09407875187294	-27.40249139272540	7.62502781056037
C	35.88331248944009	-28.51596268825865	3.64711045860520
C	31.38880125286623	-24.92479843999775	3.81098419217380
C	34.26992762925292	-23.89307363425605	9.06222729396677
C	38.25715215232067	-28.27231743884109	7.72525914305058
C	35.57505704168885	-29.07128517816854	2.33771185770599
C	31.42563547761365	-24.11251532998751	4.91323833537412
C	35.31169271199346	-24.63209846858729	9.55530603364888
C	38.36706937419198	-28.90722189414400	6.51907947454943
C	34.38762877771040	-28.50903502779501	1.95102184906115
C	32.56159868596671	-24.55162569024413	5.70890165313315
C	35.63268717723651	-25.61883933638028	8.53472314941902
C	37.26081955822470	-28.42984375715029	5.70260451136735
C	33.99529636644977	-27.60403877831303	3.02096506316536
N	36.50958016532265	-27.51875929967821	6.39257091534618
Fe	34.80018243707185	-26.63239124029130	5.79051243336716
C	33.57896639868680	-31.36314695418642	5.20220724095873
C	32.62887296155706	-32.19995699994318	6.04423981561876
C	32.52511327388251	-27.67835346637105	7.39913167848746
C	33.74260399165278	-27.91742421902333	6.55561508802078
C	34.03128768000199	-29.37594315272793	6.44363769760632
O	34.73801808732821	-29.99544271432045	7.20614112530590
O	33.36472429806479	-29.94856158166238	5.40922805380780
H	29.73729040037276	-22.82632823741918	4.52477513684182
H	31.05225416344087	-22.03954952879783	5.40398846146724
H	29.99192003222818	-23.17839451449253	6.23599889239381
H	30.92359599738846	-24.75187810454954	1.70387468090810
H	29.88030523841753	-25.87014278189794	2.58328496954779
H	29.66967349934185	-24.12744830437971	2.77939584099454
H	33.40253176005164	-27.79821121397690	0.16051513511650
H	34.13810952503776	-29.39581615422827	0.00116115629116
H	32.62878570328064	-29.20093975163316	0.89978584838993
H	36.01931282458268	-30.29354665492023	0.61671443386316
H	37.45172565827909	-29.69852843027992	1.46281389020695
H	36.50440535951070	-31.01708943433151	2.15296038669992
H	33.97487127786462	-22.49015697196041	10.67286780173187
H	32.48491410104116	-22.95323493832051	9.84407731592036
H	33.61075348471145	-21.83354950904256	9.07304115796751
H	37.09560521213583	-24.25503820251485	10.71926842390681
H	35.99130213820875	-25.42043287339648	11.45039708600972
H	39.95010255232397	-29.09790177019781	8.77505945987009
H	39.55071458841302	-27.44338166512426	9.25033864684844
H	38.54666112656123	-28.78728634951432	9.80170198213172
H	38.90941554589018	-30.88318981473681	5.83991888798821
H	39.90923456650183	-29.59182294708728	5.16662882247467
H	40.13435904600388	-30.10094851654883	6.84367914472464
H	35.59958237193308	-23.69819235604320	11.47814555080922
H	39.58979734181089	-22.87140504154276	3.76415887975040
H	38.59429338486764	-21.60813190776426	4.50966951942736
H	39.39991472190538	-22.81513650902924	5.52120506019048
H	31.58892536868327	-31.92614214067168	5.84695180987031
H	32.75115958698274	-33.26288178683455	5.81145595016006
H	32.83135721682871	-32.05941955535849	7.10749423174129
H	34.61967675339832	-31.59737141505786	5.43103217463263
H	33.40571526093027	-31.50767076974408	4.13469788870525

H	32.29741370585953	-26.62375405603290	7.53063099002074
H	31.65122917186772	-28.17282607668116	6.95028117516513
H	32.66112348886872	-28.13304627885984	8.39115241343925
H	36.88816632463910	-23.05719675251401	2.59022259029764
H	37.56086311138520	-24.77492382625357	6.36480073297252
H	35.04599238785322	-24.77488826560650	3.01916448165772
H	32.22525185589630	-26.87551609868544	2.11343685176427
H	37.24832493133145	-26.53728837634979	9.55151888923371
H	37.67231820592293	-29.60063867945014	3.98640417416188
H	32.33120422323138	-23.16866904911455	7.29866839617087

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B3LYP Scan/Melmid IPC Model/BSS/280 degrees Constrained Optimization

C	38.88697577124486	-22.69739175540893	4.57799423381162
C	37.68969524369643	-23.58773051180829	4.51361649524072
C	37.17862416740132	-24.51327104828173	5.38826030351157
N	36.81963376780602	-23.61412445487031	3.43257313313671
C	35.84661311345002	-24.52996924264318	3.69242379962720
N	36.03921133124719	-25.08831302671063	4.86709105438710
C	30.40942728437445	-24.85318789579238	2.65298240569504
C	36.01193016233174	-24.53148002858089	10.86128734492078
C	39.31764554902787	-29.96145776619094	6.04608544767745
C	33.55299418294663	-28.70362644561386	0.67085753837074
N	33.18419084956540	-25.57210281847004	5.08340751670418
N	34.78199648582090	-25.48715397729104	7.44332051326810
N	34.88153647133907	-27.61081354752640	4.01139371390290
C	32.83608634218444	-26.75539178398750	2.96753063352704
C	32.92891838006695	-23.97459048411912	6.92155104823687
C	36.64379114031363	-26.56333359836130	8.61504152240114
C	36.93852345205028	-28.88241789784903	4.38776010353901
C	30.52512228139940	-22.92513961952414	5.27423859251154
C	33.55832651689342	-22.73675838999826	9.69180542610926
C	39.06014009119292	-28.46957599082139	8.93053237531959
C	36.37221239651792	-30.05114027819316	1.57399775760436
C	32.49038001824045	-25.80558075349466	3.92545075119519
C	33.95313175131573	-24.43874822933368	7.74126943094163
C	37.05029454050619	-27.43552043248407	7.61086966035739
C	35.84016344069465	-28.50492259957871	3.62118722868708
C	31.37947400096259	-24.87439580378459	3.79751913099056
C	34.26598669490494	-23.89667751261912	9.05527128209071
C	38.20369393740079	-28.31816020963893	7.70862463946800
C	35.52731447548374	-29.05241306214418	2.30961159101900
C	31.42787271499396	-24.06318822307135	4.90005716098169
C	35.29630971846639	-24.65172389284967	9.54824218433152
C	38.31112700428467	-28.94606627063708	6.49818864963007
C	34.34260337315931	-28.48225059296918	1.92718179381005
C	32.55842291050500	-24.51807021899598	5.69475687932853
C	35.60912073700738	-25.63662223970921	8.52346900039481
C	37.21202798592769	-28.45238761338613	5.68177167969574
C	33.95793172899443	-27.57841271118279	3.00096965702424
N	36.46729928525286	-27.53918840627925	6.37644485959729
Fe	34.77046832220567	-26.62671271673467	5.77387838552154
C	33.89612176704755	-31.40970100254419	5.36727669252300
C	32.84736946848090	-32.24310031891336	6.08662328105911
C	32.46411775303593	-27.64533014917171	7.35340773440511
C	33.70659549256069	-27.90001705684450	6.55206378426617
C	34.04896474497946	-29.35123328377211	6.56273974538368
O	34.61569889025785	-29.90634129233615	7.47802665768875
O	33.60795123423532	-29.99560718732823	5.45588332199892
H	29.75575394310228	-22.75513451770933	4.51447847966525
H	31.08179415045415	-21.98575746431407	5.39241062348454
H	30.00798160415545	-23.11138139675795	6.22513354429112
H	30.91473805919964	-24.69071589873381	1.69122379654318
H	29.86080871997193	-25.80089807516217	2.56819687420126
H	29.66774083815005	-24.05683994255526	2.76935386289150
H	33.35429741844251	-27.76178376790750	0.14223973043580
H	34.08340564807065	-29.36160016080810	-0.02462189682435
H	32.57798241833762	-29.16410306039718	0.87985944727212

H	35.95956442595281	-30.27370257052811	0.58481562731910
H	37.39795007993556	-29.68736063960330	1.42695238465190
H	36.44665077422585	-31.00255125142775	2.11783570895367
H	33.98482147882269	-22.49646393548296	10.67075748120044
H	32.49007440842649	-22.94384504767068	9.84189720554628
H	33.62494943400679	-21.83149466615006	9.07343542093830
H	37.08095753317220	-24.31917531538856	10.72437393554218
H	35.94366376631238	-25.45805010974841	11.44673597779992
H	39.88803134755030	-29.16382821290293	8.75675766543869
H	39.49569071688568	-27.51199690022667	9.24676447456503
H	38.48155081681264	-28.85565177455381	9.78032357455289
H	38.84179790490658	-30.92121823394944	5.80362183275780
H	39.85272926682487	-29.63126416556054	5.14553170928103
H	40.06780901376854	-30.15629225389084	6.81901200852559
H	35.59387623070331	-23.72670319630043	11.47395024046012
H	39.59912630581570	-22.90215423144960	3.76709832902642
H	38.61637422126767	-21.63430561927066	4.52174178241993
H	39.41184906087859	-22.85513442200939	5.52469057559802
H	31.84669511736192	-32.02332562908791	5.70489223525195
H	33.04266692633915	-33.30982478441219	5.93550035200358
H	32.86512021296370	-32.04330116932845	7.15930448556628
H	34.89198007811967	-31.59090634579783	5.77420556035440
H	33.90313645235016	-31.61317546832097	4.29537545771667
H	32.19606578794889	-26.59335451966339	7.40400907030741
H	31.61538118044200	-28.20169073426947	6.92798320633048
H	32.59873847256079	-28.02497911144178	8.37615313159876
H	36.89406542430839	-23.05390577642484	2.59573812518351
H	37.55590656874539	-24.80372598937250	6.35745470143334
H	35.03643083287806	-24.75735554480034	3.01556965976307
H	32.19217865511582	-26.83426208063910	2.09713034682039
H	37.20892777010924	-26.58049282608293	9.54151379119428
H	37.61767429369628	-29.60999335335189	3.95467842128804
H	32.34384265413109	-23.13729358770106	7.28864861675736

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B3LYP Scan/Melmid IPC Model/BSS/290 degrees Constrained Optimization

C	38.92941856906704	-22.78868290915853	4.57974043941130
C	37.70915153566351	-23.64691032197202	4.51136938259214
C	37.17774410407374	-24.56833992147601	5.37815857738333
N	36.83500678688269	-23.63974458964812	3.43328215420654
C	35.83983494011548	-24.53298922343127	3.68722796531481
N	36.02234883528251	-25.10877130284196	4.85503105614897
C	30.39617184059589	-24.72373546670908	2.63452873779789
C	35.96319472694615	-24.63011207698204	10.86916587961590
C	39.23915135511449	-29.99575627730638	5.96110579991968
C	33.44951174939531	-28.64182154242978	0.63318211113704
N	33.15437156665977	-25.52562606796145	5.05809323625858
N	34.75028556562175	-25.49843214881488	7.42279921651201
N	34.80675927641885	-27.58805193975005	3.97449610272729
C	32.77308317712797	-26.69188916507870	2.94012192141985
C	32.93437481103570	-23.93818611094922	6.90892776837778
C	36.58047339430039	-26.63182244236060	8.59258001974840
C	36.85474815869275	-28.88253169951253	4.32701152266021
C	30.56857644754471	-22.80726551384914	5.26235484001760
C	33.56135865802520	-22.76341449189274	9.70626033649918
C	38.98366833726727	-28.56259489913122	8.87644705281250
C	36.25863669775695	-30.02301053565394	1.50863723439585
C	32.45299493437756	-25.73589935702965	3.90092019885837
C	33.93952030225974	-24.43943731035363	7.73071279117031
C	36.97685166344036	-27.49735825660852	7.57820400367101
C	35.75570634717758	-28.48718147026450	3.57134930995408
C	31.36689897541907	-24.77463088618746	3.77736207667383
C	34.25185153964963	-23.92597519797253	9.05589848708446
C	38.12531526332349	-28.38755575840071	7.65901335390959
C	35.43118984738601	-29.01876885422323	2.25626823853677
C	31.43914364544768	-23.96831062127379	4.88208613891574
C	35.26135945924301	-24.71073719386687	9.54578053797614
C	38.22949538089362	-28.99343008723419	6.43611665559463

C	34.24978859779334	-28.43507535909692	1.88507225077119
C	32.55723425885855	-24.45758599534841	5.67417401792697
C	35.56413689668551	-25.68457674034696	8.50799928976767
C	37.13047141203123	-28.48208055863294	5.63023262759194
C	33.88002632996083	-27.53534435283488	2.96733339720951
N	36.38838374469331	-27.58109673261331	6.34466513245590
Fe	34.71347258377136	-26.62217588564828	5.74692763838794
C	34.43932756003856	-31.42047434117643	5.80881243066634
C	33.28803527933947	-32.32988239463771	6.20762207916742
C	32.28808556540667	-27.60978248718384	7.17209175026038
C	33.62163573196639	-27.86996821837172	6.53545563361963
C	34.05291694433258	-29.27709654885692	6.77604815382390
O	34.38929684475234	-29.69011385686256	7.86548404542999
O	34.00296248716208	-30.04954250663673	5.66759544163479
H	29.80313024016877	-22.61308394802714	4.50454919273311
H	31.15106212823015	-21.88408678290967	5.38355284170649
H	30.04797205037585	-22.98335709004462	6.21327568346227
H	30.90320785236444	-24.56278666341294	1.67340219937711
H	29.82869456745863	-25.65958851607574	2.54238354682898
H	29.67045988479473	-23.91407038590454	2.75937374973143
H	33.25323783170451	-27.69496069384540	0.11271478380828
H	33.96999430128152	-29.29869691822887	-0.07070775119227
H	32.47298840282099	-29.09728012538401	0.84632187593541
H	35.84757364002469	-30.21907197303204	0.51320942783409
H	37.29324621474503	-29.68019724977736	1.37438289454199
H	36.30761790029683	-30.98588125890469	2.03527680237536
H	33.99332033373513	-22.53923003109465	10.68662742950067
H	32.49077388266271	-22.95781536728896	9.85680615140334
H	33.63883308668083	-21.85265269159461	9.09735781380476
H	37.04304977853459	-24.47023606889637	10.74779509614577
H	35.84096901784057	-25.55435308311964	11.44953571410253
H	39.80629594698386	-29.26027042597518	8.69151606165017
H	39.42685270994289	-27.61258077584410	9.20451970894590
H	38.40378868597348	-28.95543315248491	9.72219287139623
H	38.76716484897147	-30.94865644504107	5.68622070575711
H	39.77939535415628	-29.63808776428103	5.07420966638557
H	39.98451622968669	-30.21241873772781	6.73278582502845
H	35.57669622951029	-23.80775216242937	11.47926257126512
H	39.63382668772083	-23.00535837551285	3.76517117321268
H	38.68640176658027	-21.71851359293908	4.53274850568557
H	39.45262619049362	-22.96753324863628	5.52361766955897
H	32.45618252240078	-32.23788014021378	5.49999900386963
H	33.61761501808253	-33.37417509209837	6.21562989750527
H	32.92850487414736	-32.08026812535182	7.20790923047859
H	35.24685477686690	-31.45971356891334	6.54091963958319
H	34.83269720446753	-31.68047695267766	4.82470789754705
H	31.99568633775024	-26.56380203586223	7.14381449671502
H	31.50753575226717	-28.19924703610631	6.66691641414574
H	32.30305372197800	-27.95030162496201	8.21594394239553
H	36.92077699953509	-23.07274694373901	2.60210022900270
H	37.55109630526639	-24.87807535915875	6.34293303363360
H	35.02219575484561	-24.73353456602938	3.01085332997559
H	32.12592568381595	-26.75398649172367	2.07074694320233
H	37.14089752663219	-26.67069849782086	9.52114635895480
H	37.53004954776308	-29.60425619941036	3.87818691960377
H	32.36807706644204	-23.09145061194711	7.28360711638656

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B3LYP Scan/Melmid IPC Model/BSS/300 degrees Constrained Optimization

C	38.93231908321596	-22.81537218495378	4.58153543276561
C	37.71047333847071	-23.67122190578024	4.51097226852503
C	37.17533655765096	-24.59179610196583	5.37652450685330
N	36.83795176761436	-23.66133746870175	3.43162474561069
C	35.84002770663521	-24.55206366947277	3.68381631052147
N	36.01925829020037	-25.12880885803257	4.85159376947824
C	30.38054355303727	-24.71934766163875	2.63937145603717
C	35.94810015674266	-24.65981867337922	10.86951783012148
C	39.24106498164767	-29.98078679536762	5.93081172740766

C	33.42872445629659	-28.63674209123853	0.62340574297098
N	33.14653811603151	-25.52516628254254	5.05215059164726
N	34.73916304947426	-25.51009130207666	7.41735551597399
N	34.78296013424232	-27.59720286303717	3.97043957222504
C	32.74868040110285	-26.69843852847704	2.94113004985064
C	32.94555918303018	-23.92718781025450	6.89634591199434
C	36.55254027761712	-26.66521258545972	8.59275576475126
C	36.84190309491083	-28.87855713727921	4.30903804410482
C	30.58279133164512	-22.78608359814310	5.25315165903443
C	33.57899251423835	-22.75880050388260	9.69563995342939
C	38.96749581373848	-28.58511642053018	8.86256534832948
C	36.24958136971452	-30.00215695916771	1.48414483328625
C	32.43775395014632	-25.73747615051158	3.89989211950013
C	33.94245305628303	-24.43954643390810	7.72152679677777
C	36.94893530971061	-27.52756287345493	7.57550410595055
C	35.73812319142843	-28.48619789406690	3.55916113579354
C	31.35791031983736	-24.76914919597749	3.77651895086563
C	34.25643494694526	-23.93036968842803	9.04783617315553
C	38.10488302079357	-28.40881548234933	7.64814828926340
C	35.41563919463083	-29.01003259092674	2.24059336426136
C	31.44284479026782	-23.95564513459223	4.87506096010754
C	35.25187092857693	-24.73010769470065	9.54259183189212
C	38.21627614607567	-28.99978409602625	6.41821293235011
C	34.22880882593618	-28.43323201996310	1.87589934788592
C	32.56100353798554	-24.44850387538258	5.66471445220010
C	35.54576970364133	-25.70783980352973	8.50608817953342
C	37.11209442503808	-28.49166657250386	5.61740415718081
C	33.85528614736819	-27.54263903815335	2.96456561655044
N	36.36013886471905	-27.60646836371532	6.34126288296702
Fe	34.69130749104213	-26.63522280355532	5.74285214200327
C	34.54868106139906	-31.39418860042598	5.89615153120082
C	33.38583039248491	-32.32932954595176	6.18718108338062
C	32.27471121212138	-27.55980374513675	7.21865095936979
C	33.58138598007228	-27.86509243564847	6.54693972315313
C	33.99579503654907	-29.27077484684816	6.82142117761708
O	34.19186242188120	-29.69520940847710	7.94188494589289
O	34.10241283327227	-30.03232038597706	5.71069868028081
H	29.81655246113688	-22.58904200584402	4.49695125958526
H	31.17298556473215	-21.86711660454564	5.36863798962936
H	30.06391297921764	-22.95429782486948	6.20642814184543
H	30.88227389955323	-24.56340889567565	1.67462561076425
H	29.80994311792893	-25.65391264141169	2.55420996508485
H	29.65791646690493	-23.90719099830060	2.76572393750991
H	33.22000705674032	-27.68698007691042	0.11329815491568
H	33.95599958550776	-29.27980407723941	-0.08815707909675
H	32.45828117348029	-29.10645798584884	0.83337057347676
H	35.84316807742330	-30.18770481099249	0.48479938377203
H	37.28339933626200	-29.65395035722436	1.35804936470471
H	36.29985425657093	-30.97118792354456	1.99927316761126
H	34.01558862329490	-22.53535141774231	10.67411374285308
H	32.50699478634631	-22.94251640937490	9.84956754196201
H	33.66373631743111	-21.85108627422580	9.08325019720964
H	37.03197529601260	-24.52562760206715	10.75328396390101
H	35.80120904684632	-25.57829426428201	11.45333830086634
H	39.78886293197075	-29.28341244542676	8.67436866364688
H	39.41302983677392	-27.63559163110953	9.18903007550708
H	38.39077329423687	-28.97733208281164	9.71068601210965
H	38.78345186447578	-30.93433093317977	5.63499591780367
H	39.78153845868766	-29.59906196457019	5.05408348019101
H	39.98499863019831	-30.20214562228596	6.70252159500775
H	35.57772820708424	-23.82582630030082	11.47381835877688
H	39.63713726827186	-23.03248185839612	3.76743651071498
H	38.69129375196490	-21.74471186429484	4.53534975427309
H	39.45429238452224	-22.99599479617933	5.52575797264036
H	32.62102583744062	-32.25412723028568	5.40565146558023
H	33.73690768877947	-33.36604107609215	6.22411529500896
H	32.93129328833238	-32.09004824737416	7.15034959877327
H	35.28590566863404	-31.41619978770494	6.69984630984455

H	35.03716101416549	-31.64547088482250	4.95332345537410
H	31.98938149889108	-26.51430072837613	7.14849108008030
H	31.46792916674251	-28.16705769886685	6.78024370207545
H	32.33208606838210	-27.84677510614173	8.27643232866051
H	36.92621854140620	-23.09382391831934	2.60103089951590
H	37.54623784661439	-24.90232740207843	6.34205785337165
H	35.02263024069670	-24.74977543926225	3.00629666977972
H	32.09823984895856	-26.75972075415443	2.07416556524286
H	37.11071027868179	-26.70955956486280	9.52243316151741
H	37.52517077458506	-29.58712930752400	3.85135871335260
H	32.38879658364907	-23.07287119688835	7.26800247050385

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B3LYP Scan/Melmid IPC Model/BSS/310 degrees Constrained Optimization

C	38.94198658095047	-22.84948811886080	4.55749913476207
C	37.71130570709519	-23.69340033846705	4.49773029788622
C	37.17392793292033	-24.60741713076003	5.36886521230706
N	36.83160555364898	-23.67814180057920	3.42427201583834
C	35.82760931525456	-24.55949898313553	3.68522634722014
N	36.00979339991923	-25.13528879249149	4.85292254226172
C	30.35299118478996	-24.73822002294150	2.66390847049120
C	35.94407354116445	-24.65574500879387	10.87252598033539
C	39.23992236830051	-29.96712175956559	5.92767247935604
C	33.39559199072930	-28.66372139357089	0.64905152039511
N	33.13516989259504	-25.53047751840290	5.06223895336936
N	34.73341828269422	-25.51007854316116	7.42187450777764
N	34.76662567135205	-27.60190509135128	3.98173040324448
C	32.71852953345356	-26.72156365881297	2.96519405506312
C	32.95663584834382	-23.91172657287656	6.89060241896084
C	36.53455618366443	-26.67696048103155	8.60410607275982
C	36.84247235555307	-28.85922029564012	4.30580505599087
C	30.59091551706486	-22.77261752539502	5.25052952208260
C	33.60416311365637	-22.73039386457591	9.68112338263191
C	38.94684595619525	-28.60231620468790	8.87208851930106
C	36.24157120447088	-29.99192962720721	1.48671664324801
C	32.41600065750402	-25.75227800113144	3.91822105553275
C	33.94965882438058	-24.42770966781736	7.71828638374229
C	36.93221200284690	-27.53708044421145	7.58518017608004
C	35.73016670096812	-28.47813420993118	3.56299323461177
C	31.34001650489877	-24.77990551770759	3.79299232529423
C	34.26790872633120	-23.91438112758046	9.04165815030223
C	38.08993136678296	-28.41627477441737	7.65504818734175
C	35.40295634458908	-29.00742367282434	2.24782012386993
C	31.43972569898748	-23.95290825700632	4.88025397647897
C	35.25124914884176	-24.72470207319306	9.54378417540407
C	38.20993295049336	-28.99368472959872	6.41922273513450
C	34.20478091142295	-28.44761577531588	1.89353963209377
C	32.56080000239866	-24.44331845733882	5.66702618000412
C	35.53570173085295	-25.71139470896004	8.51318382344346
C	37.10729741374271	-28.48249722349928	5.61832080708556
C	33.83040052071445	-27.55905650038670	2.98361278075223
N	36.34796572921629	-27.60885378681664	6.34798497450695
Fe	34.67796913046725	-26.64104972867364	5.75194851539164
C	34.64154184241891	-31.36785408417967	5.91923653247747
C	33.45699269280860	-32.31672531257666	6.00893534028452
C	32.29022180377912	-27.52714104665043	7.28769307046967
C	33.56426236183329	-27.86928573183177	6.57153328919776
C	33.95592429168978	-29.28258240512431	6.84256094810929
O	34.01297964035575	-29.75348702002468	7.96151242290372
O	34.21370649327729	-30.00256485285470	5.72871771135757
H	29.82232318289011	-22.57733367935198	4.49630693757915
H	31.18913593191055	-21.85732836078743	5.35302990185185
H	30.07586069849721	-22.92655931144870	6.20825236340730
H	30.84660529009579	-24.59183679985762	1.69348964663095
H	29.78002852483174	-25.67241176139561	2.59216012251622
H	29.63293608257184	-23.92365173418507	2.78933615381189
H	33.17878591341255	-27.71861132079292	0.13362160278990
H	33.91987513273871	-29.30993492643949	-0.06183120960738

H	32.42886170363245	-29.13579683584996	0.87035417890671
H	35.82738563554873	-30.18659458836348	0.49229727559182
H	37.26971682257035	-29.63167309481141	1.34879297647941
H	36.30865418895139	-30.95796977473248	2.00553129229456
H	34.04691806188344	-22.50193683414966	10.65566105371585
H	32.53113609657429	-22.90248451486757	9.84118259216913
H	33.69499307649178	-21.82940619042321	9.05980113823569
H	37.03101690103999	-24.54706821292093	10.75894730842551
H	35.77432500750862	-25.56415886397113	11.46588278947805
H	39.76684954517780	-29.30204471427099	8.68335665023468
H	39.39390468019659	-27.65610865461430	9.20605918923055
H	38.36541611162611	-28.99762630407197	9.71555838109500
H	38.78650178811346	-30.91986932376357	5.62291359142357
H	39.78198310551547	-29.57661540076001	5.05585395339168
H	39.98196307038354	-30.19199212492089	6.70017226073707
H	35.59042981932090	-23.80704519244408	11.46632288552059
H	39.63973468653132	-23.07730956504817	3.74024092578014
H	38.71155396195505	-21.77666419253172	4.50809480875140
H	39.46772217434279	-23.03142752916930	5.49938058288256
H	32.81221833984230	-32.22068693369705	5.12784620948460
H	33.80799777689423	-33.35260434737047	6.06581177518738
H	32.86557076498949	-32.10950248010020	6.90294749926526
H	35.26001662317145	-31.42293592319331	6.81606644154106
H	35.25805015667419	-31.57981139643156	5.04415485700346
H	32.01968475410544	-26.47892946552086	7.20502839918121
H	31.45485391123375	-28.12914772981919	6.89883081759131
H	32.38653795752361	-27.79200006924531	8.34783972413579
H	36.91949930721893	-23.11344857449016	2.59170483755500
H	37.54860998263641	-24.91942198602491	6.33250325301368
H	35.00431332588006	-24.75211337059864	3.01335530077504
H	32.06085614997353	-26.79070986970563	2.10431219013711
H	37.08979134047902	-26.72499335344488	9.53535421216591
H	37.53289749470964	-29.55681241790922	3.84198035753658
H	32.40928727993576	-23.04861652754382	7.25580838494936

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B3LYP Scan/Melmid IPC Model/BSS/320 degrees Constrained Optimization

C	38.93992701965001	-22.85409659448148	4.55764418407618
C	37.71123140786720	-23.70067008505978	4.49439330552649
C	37.17105977436963	-24.61255414711016	5.36602302127514
N	36.83683318193326	-23.69059574354664	3.41652528848078
C	35.83329109959273	-24.57307541477870	3.67544291224345
N	36.01065026037065	-25.14455271102353	4.84595395201760
C	30.34113966478584	-24.75295112456778	2.66832706789443
C	35.93341945720938	-24.66967558436766	10.87256023566231
C	39.24242882349154	-29.96099672757167	5.91666520059565
C	33.39389721243493	-28.66693221224827	0.64381461660761
N	33.13291843558510	-25.53597477129840	5.05780824018930
N	34.73189079879704	-25.51482031815062	7.41652395650119
N	34.75888397007300	-27.60897908419756	3.98039694306414
C	32.70888974989104	-26.73282486759921	2.96551975037559
C	32.95992739734712	-23.91215306387156	6.88288720212182
C	36.52518857243816	-26.68925452216770	8.60361750154782
C	36.84458696255318	-28.85205715719388	4.29669572546516
C	30.58817355504316	-22.77854454238540	5.24753166494158
C	33.60400342755683	-22.73438817609773	9.67555337578910
C	38.93893759641355	-28.61431559902887	8.86857181629781
C	36.24959583561528	-29.97807300348795	1.47463122379840
C	32.40936731440128	-25.76153375827584	3.91731107789694
C	33.95093552687378	-24.42979142637155	7.71153481763728
C	36.92498805546825	-27.54622998085204	7.58277419433334
C	35.72869867031017	-28.47639663942647	3.55700020862620
C	31.33273956452539	-24.79004901415146	3.79353412007106
C	34.26639493342297	-23.91929752349952	9.03643349692758
C	38.08430734357530	-28.42364212282925	7.65063940694573
C	35.40424339236045	-29.00289327630110	2.24025781808897
C	31.43643896894965	-23.95935306478067	4.87772058438779
C	35.24464800356463	-24.73422737987825	9.54145163414061

C	38.20877490332941	-28.99307345374265	6.41144851987812
C	34.20169191818187	-28.45046609682234	1.88913869929171
C	32.56055088331102	-24.44685682669893	5.66186085008052
C	35.52956420850859	-25.72035673208266	8.51055869442197
C	37.10616797859085	-28.48068257666979	5.61131818344206
C	33.82246963349483	-27.56792370770605	2.98252656810837
N	36.34320187903593	-27.61352589248947	6.34422814315882
Fe	34.67241176229287	-26.64679137289546	5.74873084518331
C	34.66242360351658	-31.35730010108565	5.93384812334135
C	33.46111619788591	-32.29030663932484	5.93998969794081
C	32.34252420116807	-27.47598531395941	7.38881638415904
C	33.55487551503012	-27.86957049011925	6.59318086479688
C	33.91074247780936	-29.29331970321799	6.85007611437402
O	33.85272530815488	-29.80541925231794	7.95224620521492
O	34.27010810556420	-29.98242452967345	5.74448110095406
H	29.81741422987267	-22.58560386044474	4.49494464972439
H	31.18618715069929	-21.86271972367257	5.34613471868801
H	30.07582287371746	-22.93061544380840	6.20696993118805
H	30.83146933571516	-24.61537880988873	1.69500275643213
H	29.76479629829050	-25.68570706058934	2.60579069127358
H	29.62446443755170	-23.93497915138106	2.79071561480338
H	33.16487732248680	-27.72049287308404	0.13629109759934
H	33.92558909097261	-29.30077157998732	-0.07269667947594
H	32.43339698609970	-29.15292530251104	0.86213231922433
H	35.83713001374401	-30.17058799955101	0.47908702167972
H	37.27537603518660	-29.61030383593799	1.33899638391092
H	36.32276796859013	-30.94615837048535	1.98876231172711
H	34.04041044605118	-22.51218949921549	10.65435927043707
H	32.52897322009214	-22.90183616196985	9.82666057410514
H	33.70405012237969	-21.83136866911507	9.05861108618232
H	37.01981646290071	-24.55155814105409	10.76271759266320
H	35.76940810082284	-25.58388259058179	11.45847823958738
H	39.76537278362811	-29.30530753933261	8.67579205108716
H	39.37674068912433	-27.66757196377505	9.21293681456926
H	38.35842317949296	-29.02248409588683	9.70660067630626
H	38.79377479249187	-30.91748239126432	5.61650870645300
H	39.77711397362255	-29.56883929759059	5.04112039891452
H	39.99009842993735	-30.17907235842231	6.68568570417243
H	35.57144069342681	-23.82840710701191	11.47180837748589
H	39.64176843463135	-23.08224133411387	3.74401334791950
H	38.70742138632344	-21.7818855276127	4.50477631566665
H	39.46178911770188	-23.03277103891336	5.50229898506498
H	32.87037179196881	-32.16973919085369	5.02471280969747
H	33.79380091618211	-33.33204970299281	5.99968284948955
H	32.82313820235687	-32.08715271779324	6.80182552617439
H	35.22981261219918	-31.44042652365308	6.86216119102282
H	35.32273951260517	-31.56433773003770	5.09001991549908
H	31.97535903603534	-26.48495994772084	7.13932216947104
H	31.52501005047270	-28.19893321041580	7.26537277023914
H	32.59636213378013	-27.49012684980195	8.45687833219008
H	36.92763862778600	-23.12818891597195	2.58271195605460
H	37.54179156362834	-24.92085096297772	6.33239005981302
H	35.01335338311539	-24.76904672424931	3.00036760922545
H	32.04927748194110	-26.80361869401436	2.10630322555833
H	37.07762993785962	-26.74033058115074	9.53634568040398
H	37.53956374588431	-29.54292403590292	3.82959780512715
H	32.41408986128508	-23.04760622770710	7.24687930477103

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B3LYP Scan/Melmid IPC Model/BSS/330 degrees Constrained Optimization

C	38.93664709416652	-22.87100631982214	4.54274817723113
C	37.70586925160472	-23.71498272110787	4.48520947852080
C	37.16722566704011	-24.62486491534181	5.35988716285055
N	36.82720016374297	-23.70410474316606	3.41082835301589
C	35.82297720794813	-24.58439731536484	3.67456513427698
N	36.00375920941094	-25.15506106472807	4.84489676945801
C	30.32757744107772	-24.76195994458676	2.68597293233290
C	35.93314028794626	-24.67279174034268	10.87670041027378

C	39.24914707687925	-29.94474571720154	5.90743348458310
C	33.36994259475515	-28.68521168826470	0.66208989619950
N	33.12745989238202	-25.54236492123450	5.06668227048690
N	34.73192121499567	-25.51776250036114	7.42060825215477
N	34.74352579464278	-27.62114821624974	3.99295343374854
C	32.68697552233428	-26.75218645250153	2.98554477913811
C	32.97334793694601	-23.90285318220860	6.87961972742450
C	36.51646381541997	-26.70057746963179	8.61168807698313
C	36.84395838981698	-28.84221068915776	4.29470331409363
C	30.60411034738118	-22.76468284823625	5.24454971460867
C	33.62466687788719	-22.71981173731053	9.66816585274998
C	38.93475255884645	-28.62222031200004	8.86883391799557
C	36.24238449788821	-29.97133051723106	1.47445503935500
C	32.39612249150670	-25.77333178051824	3.93222012876857
C	33.96009715007081	-24.42463644858761	7.71054617921337
C	36.91732256754110	-27.55409317394140	7.58805942621690
C	35.71969114215662	-28.47807363742209	3.56224144676812
C	31.32521672136779	-24.79596786701650	3.80592457143740
C	34.27778450430052	-23.91254318744661	9.03405070865299
C	38.08033489876798	-28.42720208996466	7.65140142581532
C	35.39240474294050	-29.00546822353394	2.24669022128072
C	31.44132431485411	-23.95548381616415	4.88142818216978
C	35.24702926975389	-24.73529640523245	9.54414107372177
C	38.20975260034166	-28.98585311520456	6.40774688708453
C	34.18230506407007	-28.46420039345937	1.90364862002786
C	32.56578539600275	-24.44389734847161	5.66412690454238
C	35.52596114292245	-25.72652688001792	8.51662220460621
C	37.10462241180844	-28.47441913666672	5.61056160979598
C	33.80199752295542	-27.58553298434163	2.99973591544199
N	36.33700070034540	-27.61646211376259	6.34882286554796
Fe	34.66422197342322	-26.65596491125066	5.75831144522644
C	34.72035216536713	-31.34938903732558	6.00689580595820
C	33.52866930726923	-32.26980257472361	5.78990657741622
C	32.34473591423503	-27.44465382409378	7.42556317588265
C	33.53593552491766	-27.87517090974417	6.61644644920868
C	33.83786419491479	-29.31257327223466	6.86261214079001
O	33.60094693534279	-29.87140688042136	7.91890906185250
O	34.37314578667269	-29.96509539227332	5.80662986722679
H	29.83299552959232	-22.57084219461990	4.49259216489095
H	31.21022569236656	-21.85333169508467	5.33449460703360
H	30.09315131599321	-22.90515991856573	6.20646831031943
H	30.81317573685520	-24.63414049680622	1.70895632521888
H	29.74608282778024	-25.69209577545258	2.63368013553096
H	29.61588306071626	-23.93936359151808	2.80633075476677
H	33.13381778364089	-27.74001163850350	0.15549698468158
H	33.90165890493832	-29.31643998235356	-0.05667000510163
H	32.41293951366897	-29.17600904663618	0.88484576228349
H	35.82638187252741	-30.16534415772716	0.48066405777057
H	37.26403247789284	-29.59398380921050	1.33417840451697
H	36.32676473734104	-30.93966811214768	1.98627982761986
H	34.06228482341770	-22.49740985393156	10.64637293006396
H	32.54825748350189	-22.87803948946304	9.81924411235073
H	33.73242396236369	-21.82004703940057	9.04779754771680
H	37.02088989138246	-24.56572364763806	10.76907319504504
H	35.75865097950464	-25.58318391988132	11.46552941932660
H	39.76197658811831	-29.31151088377523	8.67341051727888
H	39.37139209169329	-27.67647931707466	9.21740900417118
H	38.35467942670713	-29.03451031517449	9.70517748916759
H	38.80689932203369	-30.90376248273590	5.60577703688183
H	39.77857079767341	-29.54609144599045	5.03167338870204
H	40.00044896568230	-30.15946181798527	6.67384475255267
H	35.57803407946260	-23.82585504294811	11.47205334804611
H	39.63468458750782	-23.10140151580461	3.72649118955078
H	38.70628928518394	-21.79833980901995	4.48989503304908
H	39.46192644972073	-23.05003027907573	5.48543994183209
H	33.09144758176991	-32.11305199747394	4.79713910231258
H	33.84349433546798	-33.31614685034828	5.86517616217087
H	32.76228424472082	-32.09083031549904	6.54591175692898

H	35.13257038183837	-31.47166655141582	7.00982799667763
H	35.50519370713820	-31.53533489017226	5.27132757807509
H	31.97368759158586	-26.46412837128184	7.14220731093903
H	31.52521605017331	-28.17098749440186	7.36051449329450
H	32.62572548743826	-27.40721483115804	8.48658953858385
H	36.91584468756741	-23.14259735869804	2.57616103918059
H	37.54112645692254	-24.93304267909123	6.32508008728815
H	34.99989092754356	-24.77917710368326	3.00295046981872
H	32.02280469055119	-26.82661154238027	2.13017210336412
H	37.06770767058013	-26.75437217061183	9.54498017735217
H	37.54442963564446	-29.52407883024093	3.82252477815902
H	32.43519806182878	-23.03153740815029	7.23881579845300

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B3LYP Scan/Melmid IPC Model/BSS/340 degrees Constrained Optimization

C	38.93089618286315	-22.88421894921652	4.52636018151256
C	37.69882964129086	-23.72675476304752	4.47537217607303
C	37.16165783680978	-24.63264845195404	5.35505964749314
N	36.81728594370814	-23.71929945119176	3.40330874201550
C	35.81278597629356	-24.59740438889387	3.67340670204787
N	35.99616141959365	-25.16353363707263	4.84550497004175
C	30.31227882457573	-24.78249066175842	2.70821017001562
C	35.93908289223208	-24.66282075512389	10.88010513543254
C	39.25870781459292	-29.92767493974707	5.90896312044138
C	33.34792448426751	-28.71449322788383	0.68998909595145
N	33.12131629172546	-25.55324868477346	5.08105839881673
N	34.73466653658624	-25.51690843780185	7.42732976844612
N	34.73158053517777	-27.63544160335822	4.01165992641995
C	32.66642927250226	-26.77863934741535	3.01215204943023
C	32.98530282443170	-23.89483118406633	6.87853718399020
C	36.51294444773900	-26.70338617453568	8.62289556324808
C	36.84663289126090	-28.83381241696102	4.30082166128848
C	30.61515912577093	-22.75932823659550	5.24340597745633
C	33.64696065899349	-22.69839431412736	9.65889842276964
C	38.93321304863449	-28.62315943186914	8.87683069407987
C	36.23790847978109	-29.97209431558654	1.48493726007354
C	32.38270930533839	-25.79184760644372	3.95277087608411
C	33.97070206194486	-24.41647554188608	7.71103842009186
C	36.91436797828270	-27.55531102492117	7.59794186002651
C	35.71386922542978	-28.48278262966377	3.57521177987614
C	31.31599919712641	-24.81055995261015	3.82287588886651
C	34.29161787708370	-23.89935525140375	9.03166121800541
C	38.08015106634474	-28.42497239615844	7.65894589894314
C	35.38312672401272	-29.01464464544164	2.26240621177610
C	31.44308740746599	-23.95916996144638	4.88867874457259
C	35.25382300406253	-24.72712909505737	9.54718969445753
C	38.21417078201107	-28.97590673272998	6.41233304900129
C	34.16527820094553	-28.48573888290517	1.92686459536059
C	32.56874936020025	-24.44568094494513	5.67042444057898
C	35.52671013030999	-25.72528421079289	8.52475334879089
C	37.10725936193967	-28.46609752866874	5.61669686930848
C	33.78425633976570	-27.60850445008680	3.02385283831324
N	36.33583758269055	-27.61449655579147	6.35806281422009
Fe	34.65906891673126	-26.66395481782102	5.77213581103562
C	34.74228065795706	-31.34476831513800	6.03416797600110
C	33.57931136442407	-32.22438212118043	5.59839689471382
C	32.36621112584092	-27.42141781248448	7.48427228321960
C	33.52534948179296	-27.88181287052250	6.64609497733501
C	33.77220342883455	-29.33471304712866	6.85798736761207
O	33.37289009926893	-29.94680387034119	7.83441513896396
O	34.45198691348834	-29.94546365966173	5.86083665120080
H	29.84313338761420	-22.56699834192693	4.49201630229380
H	31.22796848117202	-21.85152304468230	5.32301035390080
H	30.10620917459186	-22.88738575787449	6.20809711883290
H	30.79299237453563	-24.66548985027976	1.72743086328770
H	29.72672994232771	-25.71062337307673	2.66760000167181
H	29.60467474609807	-23.95588949014255	2.82509003435577
H	33.10401861851307	-27.77176316776704	0.18246627414878

H	33.87970795320474	-29.34435571302599	-0.02989693482626
H	32.39483008507551	-29.21012475330470	0.91856390984846
H	35.81843617015631	-30.16917309016769	0.49320350539982
H	37.25514299583398	-29.58498097178739	1.33948318792593
H	36.33408497601711	-30.93990517998992	1.99557617343457
H	34.08568922848580	-22.47389860362426	10.63612213532221
H	32.56935088855667	-22.84787573649412	9.81019655308506
H	33.76171368423177	-21.80287003142639	9.03367286077779
H	37.02761160261767	-24.56346198785064	10.77302123482938
H	35.75796342104719	-25.56918036612319	11.47314869561174
H	39.76169686044522	-29.31055232449803	8.68013058431805
H	39.36788554335812	-27.67810055067931	9.22968207278768
H	38.35261117968382	-29.03936479495942	9.71090333643555
H	38.82223226944010	-30.88894573635430	5.60592840167556
H	39.78476473422018	-29.52410187506720	5.03346403881396
H	40.01211227084311	-30.13930137762697	6.67416980856383
H	35.58904141400613	-23.81073503524495	11.47108585740294
H	39.62649649460562	-23.11883200340193	3.70923259688543
H	38.70197255108731	-21.81143632274330	4.46996660846366
H	39.45836016035588	-23.06040244500706	5.46837084610126
H	33.28759231602938	-31.99784668724778	4.56639189751638
H	33.86586437071988	-33.28023797914549	5.65050104743965
H	32.71764719059432	-32.07335551326179	6.25062842070058
H	35.00284705084670	-31.52910868253996	7.07788198459788
H	35.62124930406532	-31.51334272497316	5.40908149647416
H	32.00052593352422	-26.44064774404541	7.19431365234770
H	31.53769115723674	-28.13825526886838	7.46021062507953
H	32.67895608303145	-27.36496544850814	8.53595529269219
H	36.90444023774218	-23.16137521566826	2.56607332387763
H	37.53778699276012	-24.93750813246192	6.32043899490099
H	34.98778430824184	-24.79414483170703	3.00467405855383
H	31.99729744208796	-26.85891544990022	2.16121007986945
H	37.06356339083032	-26.75797544770560	9.55651835842800
H	37.55173618056139	-29.50842382370688	3.82512420305685
H	32.45366109647887	-23.01710391992278	7.23170134771749

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B3LYP Scan/Melmid IPC Model/BSS/350 degrees Constrained Optimization

C	38.93064026281479	-22.90598991896255	4.47568237528087
C	37.69609215672192	-23.74604100617209	4.45035271693973
C	37.16976984612062	-24.64298349020227	5.34573464108929
N	36.79917478173945	-23.74633701636715	3.39111039608723
C	35.79709786149589	-24.62004125089360	3.68323781275509
N	35.99623993836102	-25.17593690554892	4.85766611230254
C	30.27859768228994	-24.85203664694840	2.77473217365885
C	35.97460102360157	-24.61598000886537	10.88979518839626
C	39.29007186927634	-29.89754840731138	5.94230531730094
C	33.32095335183883	-28.79192977020246	0.76804778033681
N	33.12932538653424	-25.56612219671791	5.11442562637183
N	34.74950388195774	-25.50879994635543	7.45424184748471
N	34.73229927533905	-27.65772507499747	4.05902776572568
C	32.64937830046527	-26.83008533768784	3.07402764205043
C	33.00911132555280	-23.88280983765983	6.88984021854497
C	36.52953241931165	-26.68583925643485	8.65490925908381
C	36.86167299890725	-28.83127704213317	4.34046324406643
C	30.61679226848059	-22.77824448812838	5.26430566954998
C	33.69137851220277	-22.65176905643346	9.65146761412243
C	38.96232150413111	-28.58945516322407	8.90792102491351
C	36.23717947409714	-30.00420470455430	1.54108544839135
C	32.37473300695822	-25.82826763795599	4.00151797120911
C	33.99466336362802	-24.39870007503455	7.72556266560816
C	36.93010581586375	-27.54188912694829	7.63294481026579
C	35.71921887062799	-28.49841092405403	3.62120590658068
C	31.30251081618178	-24.85347050713821	3.87122239957429
C	34.32379194500549	-23.86649230662184	9.03843844145761
C	38.10304380372854	-28.40216165006394	7.69256226455242
C	35.37917472162432	-29.04941105048144	2.31857853658067
C	31.44365320146469	-23.98156814337334	4.91889811884682

C	35.28153816702523	-24.69449809292087	9.56164607410793
C	38.23816968245723	-28.95433139782832	6.44673336049248
C	34.15034037103559	-28.53941284888992	1.99222171670053
C	32.58175248050438	-24.45062340520612	5.69287169504216
C	35.54429544674342	-25.70761325057660	8.55105107788929
C	37.12444328704440	-28.45608100211868	5.65346125870817
C	33.77319541631709	-27.65231661076568	3.08278250931213
N	36.34878799451936	-27.60822399313126	6.39541189093595
Fe	34.66780703466152	-26.66947666366248	5.80947893742668
C	34.67827090363385	-31.34800799265498	5.99010277197936
C	33.62322148915059	-32.08674258988770	5.17909205898384
C	32.36257761545708	-27.39782891201095	7.51769222047427
C	33.51000961967862	-27.88208463531537	6.67692180098654
C	33.64292854906225	-29.36018636934012	6.78696350402519
O	33.02905101673378	-30.03281213335898	7.59996448371414
O	34.50513301951379	-29.92252711216024	5.90851582278188
H	29.83061728803254	-22.60431525288825	4.52321137065136
H	31.22696174981226	-21.86657228699732	5.31469358747987
H	30.12571069170769	-22.88910193725182	6.24027291544781
H	30.74095159899693	-24.75737150962147	1.78284529790518
H	29.69418432985591	-25.78172814653696	2.76680301919069
H	29.57175516928460	-24.02395980904372	2.88542896109148
H	33.05767250916853	-27.85762037910623	0.25481188697111
H	33.85263939529596	-29.42138608346975	0.04773929667127
H	32.37781712094039	-29.29851015366731	1.01334930558941
H	35.80651476999743	-30.22037542557990	0.55816502860765
H	37.24619236326913	-29.60370410086630	1.37610118668813
H	36.35551337913236	-30.96355971478910	2.06275368539137
H	34.13244925677787	-22.42041667226815	10.62604014801142
H	32.61233101698600	-22.78851885781894	9.80440833535804
H	33.81524489431499	-21.76480367874757	9.01585475379055
H	37.06235378856655	-24.51606464107830	10.77504043841766
H	35.79868925573630	-25.51663270057216	11.49298872719601
H	39.79937618709177	-29.26560039779073	8.70859489947485
H	39.38513746975074	-27.63873757661652	9.25988335359324
H	38.38992647062530	-29.01351263096799	9.74377623705632
H	38.86198507813044	-30.86428989215243	5.64467033745514
H	39.80837098403266	-29.49208805239122	5.06307593173150
H	40.04882230127897	-30.09904798575143	6.70498492067453
H	35.62701364697955	-23.75856557234366	11.47445839039008
H	39.61263697672052	-23.14861562302280	3.64947703671412
H	38.70338452660322	-21.83311384210045	4.41471765117479
H	39.47246806324898	-23.07648617668714	5.41052854107523
H	33.61639760397259	-31.73045681620159	4.14257216765237
H	33.83240704859442	-33.16181604752754	5.17458150891261
H	32.63231576313801	-31.93501057973466	5.61080759909335
H	34.65306764260779	-31.65288583572136	7.03766731502481
H	35.67881686493953	-31.52146465102177	5.58879506417680
H	32.03181394653549	-26.40013259386228	7.24471870853962
H	31.51426397534473	-28.08792541445163	7.48166802633088
H	32.67292931389838	-27.36176207074895	8.57211944114743
H	36.87547902835501	-23.19624670663704	2.54765439526394
H	37.55850728562847	-24.94005454702080	6.30856317078120
H	34.96239275729199	-24.82103479431730	3.02804417070252
H	31.96764571076476	-26.92892550348320	2.23514158093056
H	37.08378939824766	-26.73282198933871	9.58683170345023
H	37.57096327207485	-29.50108795092533	3.86417989228261
H	32.48315533140698	-22.99771653457957	7.23302153922332

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B3LYP Scan/Thiolate IPC Model/RKS/0 degrees Constrained Optimization

C	30.702704	-24.777443	2.323850
C	35.859804	-24.570236	10.820756
C	39.263646	-30.088449	6.228571
C	33.704272	-28.836820	0.613069
N	33.260873	-25.604391	4.945017
N	34.727932	-25.549195	7.377674
N	34.873986	-27.802640	4.027488

C	32.937519	-26.855099	2.865860
C	33.025193	-23.924924	6.708955
C	36.451066	-26.714103	8.670283
C	36.917833	-29.063754	4.479892
C	30.819073	-22.753570	4.871341
C	33.612838	-22.638470	9.472528
C	38.867809	-28.601937	9.096310
C	36.472358	-30.211233	1.632562
C	32.621006	-25.837333	3.760827
C	33.968808	-24.434127	7.597691
C	36.876933	-27.617913	7.701613
C	35.846325	-28.691512	3.674563
C	31.593317	-24.830338	3.530128
C	34.255528	-23.872615	8.910813
C	38.037864	-28.487506	7.851640
C	35.590625	-29.226680	2.344026
C	31.643251	-23.977306	4.599034
C	35.198214	-24.686213	9.479121
C	38.202423	-29.114527	6.647605
C	34.429550	-28.644316	1.912068
C	32.688820	-24.483791	5.478007
C	35.487249	-25.724762	8.499447
C	37.123583	-28.643165	5.789041
C	34.012244	-27.733705	2.971494
N	36.336952	-27.750081	6.455530
Fe	34.725924	-26.752162	5.747969
C	34.505641	-31.414926	5.979329
C	33.645439	-32.013080	4.873447
C	32.277031	-27.356226	7.244007
C	33.492970	-27.865912	6.513741
C	33.455985	-29.365365	6.566722
O	32.575415	-30.014183	7.116247
O	34.489512	-29.984245	5.949917
H	30.083603	-22.577046	4.078634
H	31.441683	-21.851215	4.947297
H	30.265569	-22.837601	5.817131
H	31.279889	-24.659910	1.396194
H	30.108830	-25.695830	2.214222
H	29.999653	-23.939045	2.379291
H	33.616044	-27.896059	0.052055
H	34.222398	-29.553962	-0.033021
H	32.682747	-29.212306	0.766727
H	36.082834	-30.453024	0.637497
H	37.490339	-29.819666	1.499484
H	36.565197	-31.156170	2.186037
H	34.002721	-22.401569	10.468621
H	32.523232	-22.750207	9.565432
H	33.788975	-21.762012	8.833503
H	36.948605	-24.454443	10.728190
H	35.687537	-25.461618	11.440316
H	39.683694	-29.321951	8.969395
H	39.320247	-27.640061	9.375608
H	38.270000	-28.934094	9.957043
H	38.836921	-31.050409	5.911326
H	39.850319	-29.706231	5.381663
H	39.965246	-30.297105	7.044038
H	35.484940	-23.706564	11.380926
H	33.940057	-31.609656	3.901090
H	33.759142	-33.103415	4.849216
H	32.592529	-31.781173	5.042442
H	34.173183	-31.761910	6.960626
H	35.557657	-31.674433	5.842284
H	32.198187	-26.276027	7.248561
H	31.362613	-27.774471	6.802200
H	32.279491	-27.713173	8.283058
H	32.340573	-26.915884	1.960569
H	36.978594	-26.726313	9.619640
H	37.635021	-29.765151	4.063441

H	32.490000	-23.029729	7.011285
S	36.434187	-25.254696	4.684648
C	36.049024	-23.490648	5.004549
H	35.070697	-23.209262	4.597705
H	36.046158	-23.264808	6.077543
H	36.811636	-22.864178	4.526064

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B3LYP Scan/Thiolate IPC Model/RKS/10 degrees Constrained Optimization

C	30.684803	-24.805092	2.349578
C	35.909503	-24.521261	10.805139
C	39.241949	-30.118296	6.257468
C	33.702211	-28.842442	0.630176
N	33.245125	-25.623608	4.971531
N	34.736637	-25.544691	7.388707
N	34.854304	-27.831285	4.057588
C	32.920869	-26.878883	2.894098
C	33.021630	-23.930697	6.722839
C	36.470912	-26.695804	8.678052
C	36.901297	-29.087720	4.508842
C	30.803908	-22.772999	4.890099
C	33.644388	-22.607674	9.460178
C	38.872358	-28.600398	9.112122
C	36.468903	-30.217481	1.650854
C	32.603277	-25.861473	3.788984
C	33.977714	-24.427783	7.604963
C	36.883903	-27.612349	7.716372
C	35.829242	-28.716505	3.702938
C	31.574605	-24.855807	3.556615
C	34.280427	-23.849242	8.906999
C	38.038870	-28.489685	7.869533
C	35.580133	-29.242984	2.367666
C	31.625899	-23.999211	4.622574
C	35.230987	-24.654908	9.473646
C	38.192627	-29.129392	6.671123
C	34.419888	-28.659136	1.934623
C	32.673919	-24.501453	5.500922
C	35.508442	-25.705645	8.503809
C	37.113644	-28.657126	5.813009
C	33.996605	-27.756687	2.998096
N	36.336435	-27.752062	6.474615
Fe	34.717934	-26.763338	5.771849
C	34.463048	-31.425259	6.000551
C	33.780094	-31.919548	4.731716
C	32.250931	-27.357359	7.242042
C	33.477527	-27.871177	6.532066
C	33.376631	-29.366171	6.469265
O	32.374478	-30.003526	6.765538
O	34.505481	-29.995610	6.071570
H	30.067705	-22.599284	4.097447
H	31.428077	-21.871266	4.960541
H	30.251550	-22.851336	5.837043
H	31.263202	-24.688473	1.422531
H	30.091288	-25.723688	2.240348
H	29.981632	-23.966683	2.403100
H	33.610019	-27.895995	0.079665
H	34.228635	-29.548442	-0.021451
H	32.682879	-29.227325	0.774804
H	36.092222	-30.440263	0.646485
H	37.489234	-29.825763	1.538877
H	36.552172	-31.173021	2.187618
H	34.042643	-22.360439	10.450428
H	32.555384	-22.716186	9.562895
H	33.817123	-21.738767	8.809989
H	36.996848	-24.405190	10.697309
H	35.746496	-25.405019	11.438031
H	39.683072	-29.326649	8.987615
H	39.332092	-27.639615	9.383229

H	38.275358	-28.922477	9.977263
H	38.803526	-31.078858	5.952136
H	39.828998	-29.751533	5.403981
H	39.944978	-30.325825	7.072009
H	35.540326	-23.651204	11.359182
H	34.238637	-31.467489	3.849413
H	33.869784	-33.009605	4.654009
H	32.720911	-31.659713	4.744460
H	33.959767	-31.817015	6.888445
H	35.513666	-31.722214	6.021486
H	32.313348	-26.305059	7.495133
H	31.374715	-27.498278	6.592711
H	32.034225	-27.937201	8.147488
H	32.324970	-26.938425	1.988067
H	37.006546	-26.698906	9.622929
H	37.615485	-29.793370	4.094504
H	32.487770	-23.033726	7.022241
S	36.404394	-25.277933	4.656969
C	36.057761	-23.514152	5.019672
H	35.076961	-23.207445	4.637636
H	36.079454	-23.310431	6.096913
H	36.822093	-22.891251	4.539207

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B3LYP Scan/Thiolate IPC Model/RKS/20 degrees Constrained Optimization

C	30.71470175540196	-24.79052332301577	2.29760066859588
C	35.84332421419654	-24.54574496085762	10.81350978158200
C	39.21954303058747	-30.13187015416760	6.28152240785540
C	33.75548590113718	-28.81474835249800	0.59014276728129
N	33.24595999285235	-25.62242252198622	4.94319795609356
N	34.70628378092467	-25.55355168396839	7.37992281872966
N	34.85697808539983	-27.83199243494372	4.04263759490840
C	32.94546217396937	-26.86536106845680	2.85537304570630
C	32.99584127041728	-23.94147172417821	6.70533313297329
C	36.43088259202588	-26.70804729703687	8.68089898307354
C	36.89860038935976	-29.09217640142207	4.51166576461612
C	30.79850507219816	-22.77655963089042	4.85363365575960
C	33.58269656540624	-22.63382865288353	9.45839323473686
C	38.82702368246464	-28.61570987101275	9.13397304988122
C	36.50423355609363	-30.20240222691884	1.64145042201970
C	32.61831798437014	-25.85284469881438	3.75171425909086
C	33.94228656079903	-24.44080532503407	7.59539752095953
C	36.85476512842207	-27.62049523971305	7.72012557814574
C	35.83608975369323	-28.71627219563842	3.69530787703655
C	31.59106017790780	-24.84720575647770	3.51408574254438
C	34.22894492977297	-23.86938009312546	8.90380378963086
C	38.00620517683018	-28.50088803687997	7.88338447018069
C	35.60565475163874	-29.23297177833364	2.35289103978287
C	31.62677521242967	-23.99873541779567	4.58694658299734
C	35.17711840343083	-24.67482219640177	9.47525745130431
C	38.16979460868645	-29.13964203965492	6.68590435856309
C	34.45324080735496	-28.64350790159201	1.90689523479681
C	32.66541850126686	-24.50517349801121	5.47454117556777
C	35.46800185317689	-25.71858289152557	8.50161521191359
C	37.10058253739705	-28.66287604511008	5.81776499197074
C	34.01634195812613	-27.74762881982513	2.97018574799385
N	36.32035422891227	-27.75601782679664	6.47236340740471
Fe	34.70584372004488	-26.76516828628868	5.75508686906300
C	34.43164516390523	-31.42743912302090	5.98045585142529
C	33.80761844493545	-31.88422785898453	4.66828507176254
C	32.35373388644562	-27.35024917128547	7.40002168160328
C	33.47871092697851	-27.87197183605427	6.54386203564861
C	33.35181952880905	-29.36233927161076	6.43478264061789
O	32.32438518914628	-29.99280808110315	6.64757009854955
O	34.49262693381984	-29.99979952829516	6.08839146443998
H	30.06853547740090	-22.60131703226867	4.05557388778699
H	31.41908701289831	-21.87312802538543	4.93401643517260
H	30.23835521044941	-22.86138158833777	5.79540099074082

H	31.30349749303841	-24.67037813959545	1.37760736445621
H	30.12192861626373	-25.70830362810623	2.17813465712868
H	30.01162663734551	-23.95178538265134	2.34700356121949
H	33.68395662562791	-27.86578103286745	0.04083706522467
H	34.28403817809111	-29.52544687543616	-0.05461698624683
H	32.72935645928330	-29.18761970790063	0.71686175944538
H	36.14108433345968	-30.41838914643311	0.63067011435095
H	33.52566981917361	-29.80926168864472	1.54587967276980
H	36.58104105269613	-31.16170533123690	2.17248057193563
H	33.96869904007863	-22.39217778617451	10.45487539961950
H	32.49294541961100	-22.74663121320186	9.54789235062934
H	33.75984432450900	-21.75979513832020	8.81632959299037
H	36.93035602185122	-24.41801775818097	10.71574513820348
H	35.68417096875224	-25.43621856720566	11.43789553327787
H	39.63660136841393	-29.34442489070626	9.01654501582467
H	39.28712792404997	-27.65673060468281	9.41080397721423
H	38.22056826981489	-28.93698621433267	9.99285751496833
H	38.78062218677305	-31.09041336505959	5.97059275517056
H	39.81656618590249	-29.76644325881436	5.43438044768292
H	39.91354804100143	-30.34307015928843	7.10282843360649
H	35.46103638053646	-23.68402160825557	11.37165733566900
H	34.31830270705970	-31.42427125054262	3.81972097234035
H	33.88294408245648	-32.97413680740281	4.57431447863907
H	32.75405149688910	-31.60517880002418	4.63143428356956
H	33.87746793357925	-31.83046215049468	6.83243323254694
H	35.47519377013104	-31.74154002286773	6.04936383740348
H	32.05707255322709	-26.33894737561963	7.13431067387076
H	31.48443996260175	-28.01158245103428	7.37348492884060
H	32.69370157034301	-27.30984149194576	8.44673997429906
H	32.36186923545541	-26.91827318310614	1.94099885109737
H	36.95679408540796	-26.71463570991827	9.63123848329098
H	37.61528394928448	-29.79856973458023	4.10292702172102
H	32.45514228450616	-23.04810174411624	7.00328693036380
S	36.40828036345445	-25.27839247094830	4.66950993295875
C	36.08135395838308	-23.52117256944650	5.07924260034640
H	35.10518386653414	-23.19216781554308	4.70361955757302
H	36.10262322074521	-23.34769873727301	6.16166319747158
H	36.85466016718272	-22.89461642043937	4.61827742401942

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B3LYP Scan/Thiolate IPC Model/RKS/30 degrees Constrained Optimization

C	30.72116804907095	-24.71197075642932	2.31643082211608
C	35.88931817342863	-24.56521235771911	10.81276106584899
C	39.17664090607489	-30.17538738866232	6.23967265151030
C	33.73299316814512	-28.73584901241416	0.56081063391173
N	33.24619761862117	-25.58982660279647	4.95355017069794
N	34.71434663981078	-25.55508564409346	7.38696133874285
N	34.83819390296085	-27.81105637934792	4.02808529116243
C	32.94792776878506	-26.79844109970261	2.84382010295708
C	32.99049345954131	-23.94157090706213	6.74328726903582
C	36.45626650836636	-26.71243377803426	8.66067104649777
C	36.85187815159023	-29.11409746059643	4.49341636773344
C	30.78576743495577	-22.75405030095421	4.91590932463459
C	33.60011055460690	-22.65662572169485	9.50150767145686
C	38.84108338746807	-28.63765526219337	9.08863590840268
C	36.43304134880414	-30.20849378994306	1.61908182530045
C	32.62228145817932	-25.79889904691145	3.75610637346569
C	33.94678506827701	-24.44744837899739	7.62015568793303
C	36.86298447731338	-27.62627319328940	7.69465275596013
C	35.79589960755808	-28.71779281727365	3.67836973634517
C	31.59302076582536	-24.79136316684625	3.53486628713222
C	34.24617991152810	-23.88455938069438	8.92995134360039
C	38.00501199850144	-28.52040297188411	7.84849886319477
C	35.55909666201980	-29.21778484368388	2.33087629000310
C	31.62148145119746	-23.96578134389618	4.62588961841844
C	35.20675272530477	-24.68819450768614	9.48232692502866
C	38.14527279539098	-29.16774883561162	6.65281844600587
C	34.42695482266519	-28.59334523456999	1.88277367438369

C	32.66004653122111	-24.48550984671466	5.50502462831791
C	35.49009245896874	-25.72380898571879	8.49795179584046
C	37.07327501373528	-28.67918328342110	5.79486811458453
C	34.00456999276101	-27.69764432876775	2.95169042131267
N	36.31365651140636	-27.75829342230931	6.45278734181199
Fe	34.70507426062689	-26.74964038775229	5.75086171776987
C	34.38168403888665	-31.46623352637330	6.32686270439640
C	34.24884203449049	-32.00995031849374	4.91110894617953
C	32.20616566364378	-27.36598228918763	7.15738954878716
C	33.45379080147971	-27.86523628723144	6.47138124481028
C	33.32114733235600	-29.34358878719688	6.28733014845699
O	32.25290190838856	-29.91584911080307	6.13697716095009
O	34.48354855908050	-30.03481097549644	6.36617624708847
H	30.05454152125273	-22.56807025136104	4.12139355100201
H	31.40025698490799	-21.84817138294350	5.01381638581249
H	30.22609943514318	-22.86077113709896	5.85575296724928
H	31.31298225103409	-24.56833851392698	1.40169970184221
H	30.13357454289277	-25.62976071298958	2.17389342528440
H	30.01371914098755	-23.87797850389433	2.38162336837520
H	33.68099475315645	-27.77883547391209	0.02346708384310
H	34.25251204001076	-29.44724667401897	-0.09043699424166
H	32.69980194195966	-29.09225071312181	0.67783698169733
H	36.07218556722612	-30.40496842850002	0.60349300185840
H	37.46719668211296	-29.84703700546907	1.53517599430613
H	36.47565342564866	-31.17465482435301	2.14198657952524
H	33.99775910395059	-22.41980660093707	10.49456868591267
H	32.51217581131058	-22.77588103440205	9.60429069481539
H	33.76402912938919	-21.77708233690775	8.86342292009204
H	36.97475283465997	-24.43502454342653	10.70186087682232
H	35.73974590945477	-25.45956243876009	11.43403025815013
H	39.63997366112909	-29.37714851624294	8.96519294576943
H	39.31699501111439	-27.68271763526962	9.35244660655077
H	38.24264699008787	-28.94536264446236	9.95801375326826
H	38.72034126087089	-31.12748114763710	5.93420026523559
H	39.77071182599604	-29.81978793845486	5.38621700752213
H	39.87573639651476	-30.39554993909012	7.05431761371480
H	35.51252958838830	-23.70729365451038	11.38052269893462
H	35.07935757441294	-31.66986201910628	4.29013368095398
H	34.24968776968255	-33.10638135348382	4.92915424545459
H	33.31663226626472	-31.67087766213668	4.45906145833051
H	33.53167782241594	-31.78039880648345	6.93864554122910
H	35.30665151034766	-31.81037291625357	6.79482821182355
H	32.33398494577122	-26.37765189084106	7.58837159426336
H	31.40294305563417	-27.30052793446432	6.41047076480017
H	31.84177640953823	-28.05666566292767	7.92803038363000
H	32.36774005297291	-26.83192925078613	1.92635296172249
H	36.99380579323535	-26.72238832421466	9.60445586397057
H	37.55304922788417	-29.83513446264097	4.08315952629272
H	32.44752456898131	-23.05523402611314	7.05769508624158
S	36.41846203863897	-25.26490167055034	4.68629722990766
C	36.03971917450183	-23.50346375507448	5.02991966665152
H	35.06328381202142	-23.21192654038319	4.62540891839201
H	36.03665775092843	-23.29246331165868	6.10602306811673
H	36.80567317953217	-22.87323672873650	4.56162231909047

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B3LYP Scan/Thiolate IPC Model/RKS/40 degrees Constrained Optimization

C	30.73447715900762	-24.66809111651106	2.30474695159188
C	35.89532377379928	-24.57132903976887	10.80799037661733
C	39.15073939158456	-30.19509254800444	6.22593827776951
C	33.71791477613836	-28.70957389408784	0.54593253838093
N	33.23922748531308	-25.57722939068526	4.95036521679246
N	34.70368646836987	-25.55929165460458	7.38715141435266
N	34.82646669635108	-27.80120504321680	4.01641952443036
C	32.94838749364774	-26.76815547309167	2.82971184046282
C	32.98011416590957	-23.94230418772055	6.75151673081633
C	36.45555579738050	-26.71407790931079	8.64931576574365
C	36.82536901021766	-29.12552553757486	4.48433707144399

C	30.78758002201634	-22.73387693894466	4.92230783344781
C	33.594370968888560	-22.66650517804838	9.51207094893949
C	38.83780513752929	-28.64282005438307	9.06906179496987
C	36.38976385575106	-30.22533642308041	1.61344748860473
C	32.62238602244632	-25.77380850440719	3.74723654192610
C	33.93594478981200	-24.45314974898262	7.62587373764621
C	36.85795884641325	-27.62725875495695	7.68109159660425
C	35.77347636319762	-28.71973475772172	3.66809303399036
C	31.59794626624448	-24.76090283676162	3.52807411723745
C	34.23968619579255	-23.89250428009663	8.93556704132723
C	37.99632850107579	-28.52640285617100	7.83252121843193
C	35.53229526968841	-29.21748310112227	2.32061406750037
C	31.62136572732066	-23.94552538337627	4.62666508305594
C	35.20502658769381	-24.69470244493315	9.48159337743023
C	38.12719225124971	-29.17959686858648	6.63907556481619
C	34.41023804657599	-28.57698108618687	1.86976751604271
C	32.65331302399952	-24.47609216177843	5.50737228568131
C	35.48546238403469	-25.72795237520655	8.49381085300879
C	37.05418576675309	-28.68789552157411	5.78389128747974
C	33.99643603384617	-27.67692035125627	2.93809729016976
N	36.30380541485156	-27.75894610069122	6.44112653447602
Fe	34.69834965847672	-26.74380098098558	5.74310577936231
C	34.29627421089201	-31.48340039188885	6.39579276844300
C	34.45958005239135	-32.02344271806756	4.98249589358565
C	32.20843833595512	-27.40319040254096	7.16764562661798
C	33.44884460076388	-27.86340491020698	6.44456124212308
C	33.30789571361627	-29.33149913197274	6.18928313306526
O	32.26608276677009	-29.86687365226225	5.85080142394349
O	34.42292311429392	-30.05287387670248	6.46262840809886
H	30.05934737514282	-22.54080641135565	4.12671062612246
H	31.40372690286633	-21.82998029310513	5.02830968241626
H	30.22458311288375	-22.84558269902281	5.85960664167239
H	31.33273218267638	-24.51727261076953	1.39537123924161
H	30.14592696790126	-25.58325523523455	2.14980146627129
H	30.02844308728472	-23.83311912783780	2.37299519878107
H	33.68048104880751	-27.75160616388137	0.00906468620827
H	34.22951131155718	-29.42763247125748	-0.10428179735491
H	32.67971165649507	-29.05185961809907	0.66022031585725
H	36.03786879487085	-30.40541332649604	0.59166369052174
H	37.43422294108615	-29.89119414557136	1.54575758322237
H	36.39851131605199	-31.19549367367676	2.13056124365843
H	33.99629812973491	-22.43047897093791	10.50362068931065
H	32.50705177072217	-22.78742662922626	9.61970905112327
H	33.75395775936424	-21.78568293941346	8.87463165684777
H	36.97968123197410	-24.43774735034442	10.69058638104362
H	35.75246529746625	-25.46674849145390	11.42935220621479
H	39.63448941796609	-29.38439541500804	8.94383204482766
H	39.31702983496809	-27.68830413686114	9.32833330935985
H	38.24279179785574	-28.94699261806888	9.94204638629197
H	38.68867013644690	-31.14952700811051	5.93654459939684
H	39.73659664592657	-29.85113168704284	5.36214574649630
H	39.85817353799693	-30.40808836145165	7.03531453708979
H	35.51956393947759	-23.71509456641159	11.37903738377505
H	35.41179007351594	-31.70169071079220	4.55766385368223
H	34.43312873107950	-33.11963431336549	4.99573740963417
H	33.65546260231838	-31.66336296338790	4.33983151245304
H	33.32693538928410	-31.77473762779771	6.80841427621076
H	35.09032009819394	-31.85061793366643	7.04992150050008
H	32.24162518414416	-26.35618385771394	7.44900936210247
H	31.34119516546088	-27.56994213850675	6.51603837335057
H	32.02220789740240	-28.00595902896314	8.06959621408212
H	32.37223637151737	-26.79286738154712	1.90943239605706
H	36.99788127633830	-26.72426697129329	9.59037742823710
H	37.52022775292291	-29.85281318584067	4.07430731162644
H	32.43798791932602	-23.05694679813014	7.07019377848391
S	36.40435178263691	-25.25436252237231	4.67229005334110
C	36.04773410426886	-23.49639028621340	5.05778753483299
H	35.07034238812598	-23.18577141280891	4.66996492493156

H	36.05880237971476	-23.30770968252489	6.13791980794653
H	36.81520322516837	-22.86443174696669	4.59419490370400

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B3LYP Scan/Thiolate IPC Model/RKS/50 degrees Constrained Optimization

C	30.75632281377581	-24.60640798991933	2.28057359864256
C	35.88500063593638	-24.59869198824207	10.80495153118236
C	39.11558669639695	-30.22536317599737	6.20045571851621
C	33.70457541514195	-28.67392222268273	0.51597001608263
N	33.23893917022544	-25.55574053090777	4.93298324178305
N	34.69485467500941	-25.56179570434117	7.37634436647886
N	34.82687925793896	-27.77265750162239	3.98335992155092
C	32.95946323205013	-26.72067810856442	2.79684608060579
C	32.96542006820884	-23.94608594294377	6.75538184413363
C	36.45188040481156	-26.72127975064727	8.62696780241595
C	36.80513391505919	-29.12590054757583	4.45590340159619
C	30.78589109544445	-22.71304490221400	4.9278500063827
C	33.57184412327526	-22.69533423148711	9.52925606919706
C	38.81889633933911	-28.66901813666317	9.04324968637216
C	36.34849280884083	-30.23344088631318	1.59053916610433
C	32.63138571696537	-25.73472969405216	3.72256353317416
C	33.92153542535897	-24.46245278885889	7.62621745055863
C	36.85289863845801	-27.62970189987148	7.65372209512083
C	35.75978098560548	-28.70678330234461	3.63787001789708
C	31.60912246640515	-24.71823831416561	3.50972315221215
C	34.22306012877260	-23.91259988339275	8.94096217511592
C	37.98185652185575	-28.54049960927827	7.80491300453612
C	35.51090056355086	-29.20513864928417	2.29192773961752
C	31.62252436760265	-23.91998047012630	4.62092000335475
C	35.19393754748045	-24.71405220962215	9.47821041985434
C	38.10644778902362	-29.19477056388433	6.61134701498459
C	34.40040829848325	-28.54691550688466	1.83844277351103
C	32.64774273921420	-24.46331524866576	5.50180942793177
C	35.47879026610224	-25.73665184014974	8.48053157758347
C	37.04038814649570	-28.68977781747877	5.75522871741228
C	33.99894331273450	-27.63904165970936	2.90478431435225
N	36.30020227202926	-27.75298000930493	6.41210792173352
Fe	34.69847706101803	-26.72851809325112	5.71700855246632
C	34.28677341220214	-31.48389420110608	6.52682411502435
C	34.59787534351192	-32.05724393077822	5.15206442657328
C	32.22759376571015	-27.44036680649386	7.16117369088854
C	33.46254788409967	-27.86401244471370	6.40850957331547
C	33.35424725963476	-29.33080717232944	6.14087747546985
O	32.37382713600337	-29.86261591066061	5.65239960774190
O	34.41516530686043	-30.05160711939754	6.58281017368019
H	30.06154207784431	-22.51057177350570	4.13103284392731
H	31.40039529744239	-21.80983046627224	5.04860535439624
H	30.21821522550904	-22.83733144758949	5.86073891537722
H	31.36262134853156	-24.44211469617693	1.37890012281196
H	30.16879199315231	-25.51881328318286	2.10659464757615
H	30.05011131511898	-23.77214682585976	2.35545765828129
H	33.67241341321076	-27.71532920835689	-0.02008834441300
H	34.20974910498477	-29.39505298841695	-0.13584536282565
H	32.66432218559959	-29.00912729694461	0.63273192746000
H	35.99941621087493	-30.40488249678490	0.56628643287111
H	37.40144301054895	-29.92563803883638	1.53003074594276
H	36.32899741371595	-31.20310057028876	2.10817861272397
H	33.97452969798373	-22.46518547507753	10.52189505325768
H	32.48541112190276	-22.82324633834750	9.63813219215996
H	33.72501732061546	-21.80826670963300	8.89891438546751
H	36.96891285116868	-24.46169284499539	10.68759812564775
H	35.74485488023297	-25.49890804092534	11.42003770580689
H	39.61292186386135	-29.41302743412810	8.91565101004969
H	39.30105972585550	-27.71825874520837	9.31058172870451
H	38.21972024142445	-28.97668253024885	9.91221536035250
H	38.64089230871624	-31.17787024758121	5.92485938024305
H	39.69833746462639	-29.89713565726713	5.32857431168668
H	39.82696108442281	-30.43786819454320	7.00651261860718

H	35.50768427797460	-23.74747548332277	11.38248613209515
H	35.58837413186878	-31.74160967442370	4.81960836668947
H	34.57380398946498	-33.15289531186794	5.19140703604127
H	33.86365362577263	-31.71822071108670	4.42090378651967
H	33.27625232513578	-31.76205143212478	6.83829372044975
H	35.00193690995641	-31.84078116431295	7.27133217212303
H	32.19354058250178	-26.37504369294437	7.36344590163799
H	31.34044532431112	-27.72840972567606	6.58319112388763
H	32.15253145246155	-27.97921864032367	8.11932094713726
H	32.38710574155468	-26.73549471381465	1.87398491477249
H	36.99399232940997	-26.73822773296657	9.56807898942298
H	37.48980114324955	-29.86347820062118	4.04718437615949
H	32.41893953755313	-23.06658036400851	7.08280348182471
S	36.40957307105211	-25.22780339705522	4.67769837117042
C	36.03635382992856	-23.47300654533957	5.06289820353739
H	35.06163619677937	-23.16733820859447	4.66457788089844
H	36.03450797568682	-23.28596029527000	6.14334746488371
H	36.80510407636040	-22.83554673014907	4.60897471122601

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B3LYP Scan/Thiolate IPC Model/RKS/60 degrees Constrained Optimization

C	30.78083565794457	-24.52680226088675	2.25518250665912
C	35.86773478769017	-24.66603481695047	10.80350478247045
C	39.09582453731249	-30.24154921103030	6.13322656258073
C	33.69689659438581	-28.60119985306968	0.45833589766318
N	33.23618522264275	-25.53540726019659	4.91155107086686
N	34.68378065607727	-25.57867079818716	7.35914817155785
N	34.81489417812158	-27.74850228007313	3.93925287097432
C	32.96721886306911	-26.66201012346223	2.75365647314558
C	32.95292624430421	-23.95672241441398	6.75992980122237
C	36.44353765709288	-26.75199066055282	8.59340067624336
C	36.76767041648217	-29.13995934428500	4.40967466662042
C	30.78906891851040	-22.68703280419146	4.93978660910983
C	33.54725117320327	-22.75221268555939	9.55662419620451
C	38.81410467306019	-28.69942123939023	8.98462894800479
C	36.29961328309526	-30.22561659124815	1.53906620316167
C	32.63837840896293	-25.68925037441964	3.69276179236009
C	33.90693258528650	-24.48615782171901	7.62537807825056
C	36.84132649279838	-27.65237901859053	7.61125804852887
C	35.73090750022664	-28.69896906845336	3.59232906212239
C	31.62131817947388	-24.66552484861785	3.49002233938526
C	34.20487861089826	-23.95647772432431	8.94924447287547
C	37.96864378252624	-28.56632765567672	7.75254907101824
C	35.47912749829825	-29.18456311884464	2.24201249488022
C	31.62628843177901	-23.88938300397903	4.61680311598511
C	35.17883353376843	-24.76215843460574	9.47416634406183
C	38.08436813133956	-29.21776022511825	6.55637117177811
C	34.38603007499679	-28.50008171808397	1.78651400265049
C	32.64309885829869	-24.45166687779789	5.49552377726464
C	35.46815830102534	-25.76799585619015	8.46082904352282
C	37.01384826235726	-28.70782926453313	5.70879098013153
C	33.99498127510932	-27.59352717136968	2.85803188288509
N	36.28250494104039	-27.76824122727702	6.37160968962442
Fe	34.68887596737601	-26.72399352158856	5.68409942376900
C	34.24972630319530	-31.47233060722856	6.75188788140497
C	34.82184886941458	-32.07648708358373	5.47859357147828
C	32.21294625813087	-27.45976413362527	7.11643597986737
C	33.45817806046723	-27.86597796540093	6.37137401865602
C	33.39082179403774	-29.33929701158934	6.14335408734741
O	32.50426329471750	-29.88778901276561	5.51693787878681
O	34.36219314960439	-30.03714038085950	6.78705090593869
H	30.06804242389549	-22.47157455377053	4.14335119962739
H	31.40329010530721	-21.78602020386386	5.07748834834175
H	30.21757567037782	-22.82613714323054	5.86823069787388
H	31.39587573839027	-24.33899761546943	1.36401239493571
H	30.19826815636486	-25.43655774729439	2.05311185596474
H	30.07115362984507	-23.69672542128843	2.34272807579170
H	33.69995502465956	-27.64056320524138	-0.07522458910625

H	34.18357723734587	-29.33650947071901	-0.19169568970726
H	32.64550082060296	-28.90268828214877	0.56636344201342
H	35.93738076742383	-30.40180873061377	0.52019378020976
H	37.35483358665316	-29.92829350343871	1.46422341504811
H	36.27716680264650	-31.19045920969062	2.06521530606638
H	33.94793440500106	-22.53605336657433	10.55321282874027
H	32.46135094496086	-22.88735711627443	9.66237776411612
H	33.69635300044540	-21.85425799243897	8.94086166702563
H	36.95141537620612	-24.52429662007733	10.68972057014048
H	35.72938488918381	-25.57655211921813	11.40364083616314
H	39.60722954735005	-29.44297579777292	8.84901002580140
H	39.29792102484779	-27.74963095304584	9.25214662355934
H	38.22068558497310	-29.01044378128388	9.85633624568736
H	38.62689538408025	-31.19601857902916	5.85444982060876
H	39.67120979966444	-29.90423367863943	5.25995629116260
H	39.81328605896092	-30.45460271496793	6.93369556634324
H	35.48727668490851	-23.82526813468129	11.39416126746944
H	35.85798420368419	-31.76423658730859	5.33785780326384
H	34.78851169623068	-33.17101540351873	5.53590675654721
H	34.24500415733903	-31.75414522318984	4.61131829845612
H	33.19876564128409	-31.74910547280365	6.86962829646698
H	34.80874062802611	-31.80372594514345	7.62995454377483
H	32.14072871329393	-26.38927829909779	7.27953872694108
H	31.33240835629833	-27.80015972952803	6.55574670093390
H	32.16716618085037	-27.96518950172741	8.09457341998405
H	32.40181450065875	-26.65866187499432	1.82639181725106
H	36.98792195267642	-26.77831177176964	9.53296133173974
H	37.43934473734755	-29.88816172024206	3.99880196833683
H	32.40438547109409	-23.08323082546931	7.09977602953900
S	36.41604422248329	-25.22018991509807	4.68416566460422
C	36.01350452661262	-23.46515253971295	5.03922910058851
H	35.04492923422119	-23.17535291623912	4.61501987249054
H	35.98552714009521	-23.26451624620292	6.11686882073476
H	36.78512123058704	-22.82461471744100	4.59450895941136

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B3LYP Scan/Thiolate IPC Model/RKS/70 degrees Constrained Optimization

C	30.76869136562036	-24.53627151316839	2.26493547638948
C	35.90441131254185	-24.63637663318297	10.78539085564499
C	39.08726411921055	-30.25732083659472	6.13686826834306
C	33.71490773239874	-28.58043735869733	0.44789810411667
N	33.23908145571552	-25.53210808323454	4.91185618683269
N	34.69157316601086	-25.57486561786878	7.35767715588479
N	34.82431531447293	-27.73965335808102	3.93407696964631
C	32.98157822409327	-26.64756484512136	2.74676860362955
C	32.94254438312710	-23.96757169179522	6.76955043950710
C	36.46778799073864	-26.73305543820674	8.58280527698819
C	36.75778035608467	-29.15417160209289	4.41502213425170
C	30.75415067465070	-22.71745909055767	4.96366111478335
C	33.55266869267194	-22.74948720475500	9.55609223163447
C	38.83680288974619	-28.68161725445559	8.97254481733970
C	36.29860956059922	-30.22805243814435	1.53849709921000
C	32.64315060016990	-25.68426884485730	3.69187641374722
C	33.90802641772157	-24.48773173780339	7.62786612666672
C	36.85626606589183	-27.64234856271251	7.60517782681113
C	35.73158195788606	-28.69992705831516	3.59177623679840
C	31.61299682352877	-24.67207345382046	3.49752012830530
C	34.21429779064965	-23.95070116594466	8.94685922347630
C	37.98059368848066	-28.55954540419604	7.74670803879127
C	35.48278701521296	-29.18168974235497	2.23935565236797
C	31.60803395904326	-23.90514300517220	4.63056501688019
C	35.20110804549279	-24.74535775683178	9.46456800340731
C	38.08251444875528	-29.22581498773896	6.55734084591715
C	34.39888463029327	-28.48626188865112	1.77912593928696
C	32.63302993445029	-24.46066878401278	5.50427578456778
C	35.48770911101884	-25.75351207215617	8.45276160763681
C	37.00879543533852	-28.71870572659617	5.71214194177960
C	34.00967323784183	-27.57862945771597	2.85035912987564

N	36.28731925227381	-27.76776995625899	6.37073001663916
Fe	34.69711904133023	-26.71767310693208	5.68035030869112
C	34.07435457847251	-31.50032587657747	6.71266499131256
C	34.88905258859625	-32.08405444582433	5.56923834366583
C	32.23580158094725	-27.48217669539731	7.13478927580720
C	33.46246069370291	-27.86269960058651	6.34755928580237
C	33.37983481747010	-29.32072851615009	6.05139162181839
O	32.58350410266276	-29.81258662973139	5.27792578793374
O	34.21949476311515	-30.07103924764115	6.81558754025264
H	30.02946295730291	-22.50618180335093	4.16940846536438
H	31.35540918804336	-21.80873366422042	5.10788586021977
H	30.18536710928554	-22.87182146667215	5.89140275113566
H	31.37918070460266	-24.33063557828942	1.37454884905431
H	30.20104837330546	-25.45381636075318	2.05578307863137
H	30.04546373632570	-23.71887094566742	2.36058272816173
H	33.72602662563824	-27.61888892953002	-0.08386691892016
H	34.19953572683969	-29.31774046791897	-0.20142847882573
H	32.66136435843082	-28.87579183208191	0.55164464357134
H	35.94334562557209	-30.39558664490811	0.51573891944416
H	37.35734945854780	-29.94098624441301	1.47413994972935
H	36.26239734612641	-31.19553009442036	2.05913097910261
H	33.96138759110880	-22.52602863659039	10.54780885836551
H	32.46901164776162	-22.89320214446181	9.67316790015219
H	33.68811717770432	-21.85278614598203	8.93539251828740
H	36.98509685976546	-24.48347688556314	10.65822935581485
H	35.78304967030448	-25.54567740490251	11.39101786094041
H	39.62614585351540	-29.42943820334999	8.83837316135592
H	39.32631455453798	-27.73045279594373	9.22439511226479
H	38.25043676347844	-28.98027610866993	9.85327556745446
H	38.61283159324118	-31.21126951043060	5.86593640755140
H	39.66083350216161	-29.92848052171583	5.25913903742889
H	39.80685050465988	-30.46851730720074	6.93591761157030
H	35.52189045807301	-23.79716252440492	11.37694493427038
H	35.94424406859508	-31.82550782140608	5.67620006468046
H	34.79420013573906	-33.17643570232296	5.56081867132444
H	34.53726612902155	-31.69456240710378	4.61325654741862
H	33.01538186080978	-31.74177873985240	6.59425179898587
H	34.42232458243878	-31.87677935314099	7.67754161857482
H	32.18415287761540	-26.42128349172951	7.35920112213318
H	31.33791857223780	-27.77468061333814	6.57300390864630
H	32.20292571896320	-28.04228036574548	8.08296862700799
H	32.41805120561097	-26.64196043957264	1.81839718195590
H	37.02069509165492	-26.75135981930564	9.51756211101248
H	37.41976065088132	-29.91329594081532	4.00888793429658
H	32.38663057477502	-23.10083636160748	7.11469320429023
S	36.41183046727787	-25.20942311103392	4.66930235113888
C	36.01836304967601	-23.45917186075251	5.05743893432505
H	35.04496172768467	-23.16101895974855	4.65034946291152
H	36.00509906322680	-23.27465429940058	6.13820761640273
H	36.78520570442942	-22.81345190174663	4.61190427632870

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B3LYP Scan/Thiolate IPC Model/RKS/80 degrees Constrained Optimization

C	30.81275865500292	-24.37811125739505	2.21636437570287
C	35.84581102706588	-24.81964457084679	10.78571122351293
C	39.03996317381676	-30.297933557975051	5.96860798346635
C	33.69119508752025	-28.43185678567860	0.32091905322232
N	33.22722848809676	-25.50294958390833	4.86388568612934
N	34.66212046687355	-25.63030984936981	7.31621820795555
N	34.79542401576995	-27.69571950162426	3.83287806524493
C	32.98032115361816	-26.54341869725850	2.66063301643567
C	32.92716677865728	-23.99435431786246	6.76721907031890
C	36.42663959191066	-26.83599980638721	8.51335180119895
C	36.69179646926480	-29.16640661628158	4.29083022344406
C	30.78736591240343	-22.64924748916611	4.97307761696948
C	33.51050706496684	-22.88328422681592	9.60288036377260
C	38.79831089554845	-28.79323879944868	8.84663080084612
C	36.21408515095869	-30.17905481073354	1.39877140624221

C	32.64589647703419	-25.60448472153240	3.63203587592607
C	33.87899030888028	-24.55219281641077	7.61776573682783
C	36.81340762692880	-27.72065896812149	7.51231776124269
C	35.67897542709962	-28.67209542193632	3.47576374107472
C	31.63493314381041	-24.56990322444214	3.45635782989482
C	34.17534187835009	-24.06342752496153	8.95745179026199
C	37.93381020121028	-28.64546345893333	7.62937744432877
C	35.42652491114730	-29.12006408549740	2.11193932027020
C	31.62595470171923	-23.84028395649961	4.61387322133757
C	35.15617787392707	-24.87812829856591	9.45465507471137
C	38.03031499129203	-29.28529895887867	6.42367677931440
C	34.36675373754742	-28.38626386871892	1.65893775857642
C	32.62983820309153	-24.44012008332585	5.48219557574321
C	35.44963603389300	-25.85048939406318	8.41046398146854
C	36.95425997549698	-28.75666345944528	5.59526567683045
C	33.99145989314204	-27.49341595557883	2.74861223204625
N	36.24143864945174	-27.81534361246099	6.27621395472517
Fe	34.66840020722131	-26.72477373564686	5.60785554922113
C	34.15209718318290	-31.38923280919350	7.21914941576726
C	35.30707843435432	-31.99413316353112	6.43801124478413
C	32.13855357846970	-27.52234773658094	6.92658269097635
C	33.44133524136566	-27.88322201295406	6.26262131694266
C	33.49754037424286	-29.36530276816945	6.13588908714390
O	32.93554749776099	-30.00443354925937	5.27214898642123
O	34.16680272057428	-29.94990412397624	7.17022408750518
H	30.07111454820624	-22.40678691963338	4.18011896771142
H	31.40098672178522	-21.75357794969091	5.14451830125681
H	30.21057988589660	-22.81948364127591	5.89299853331763
H	31.43954705198828	-24.13995791016791	1.34549750826342
H	30.24322216425651	-25.28224756485496	1.95956443948247
H	30.09294486818645	-23.56049590518196	2.33347428115019
H	33.74095214583424	-27.46202443683696	-0.19359535338679
H	34.15438211642886	-29.17461188524855	-0.33778233504341
H	32.62681478480988	-28.69084143691579	0.41062604963604
H	35.86728314028730	-30.31195432764622	0.36803620818638
H	37.28338899574069	-29.93001394206936	1.35439083913875
H	36.13450010963100	-31.15494371444814	1.89838267527261
H	33.91207692524884	-22.69393931071160	10.60455206261785
H	32.42584427211630	-23.02957746149251	9.70705206061268
H	33.65122304543340	-21.96594883613815	9.01423250673310
H	36.92963261011145	-24.67683751263293	10.67489318211814
H	35.70629559364331	-25.74608726400280	11.36068247424831
H	39.57447151910618	-29.55221089130149	8.69872472908584
H	39.30473846755005	-27.85232534272489	9.10330175843347
H	38.21424162093550	-29.09108477499056	9.72892786172557
H	38.56942017165989	-31.24327012247080	5.66363172927812
H	39.61179483512529	-29.93418841062607	5.10369911000096
H	39.76002911194989	-30.53345265580607	6.76038389137228
H	35.46738783768824	-23.99457766929148	11.39943145688718
H	36.25951213926490	-31.60002048469295	6.79814545829801
H	35.30895157450330	-33.08482576038796	6.55071287506283
H	35.21778650095980	-31.75233276018486	5.37798519502719
H	33.19317873302407	-31.74854539861377	6.83910431178926
H	34.22843716000275	-31.62648511393983	8.28327719971756
H	32.01787307784753	-26.45358105045759	7.07728703880679
H	31.30574038179309	-27.88882393047187	6.30852067476152
H	32.04761540968136	-28.02970786199033	7.89953649141573
H	32.42731066070944	-26.50135634960687	1.72687536305185
H	36.97638260526054	-26.88367018410524	9.44891103857528
H	37.33749387358753	-29.93185514743836	3.87091173264769
H	32.37528060885547	-23.13468122103279	7.13571280680587
S	36.41915501846682	-25.20734232204084	4.67883615051527
C	35.97240211237522	-23.45599296357136	4.99883462999980
H	35.01710328599570	-23.18668609856366	4.53317414144416
H	35.89838141044248	-23.24461980927803	6.07219741459959
H	36.75024638594068	-22.80713415625202	4.57758391758063

B3LYP Scan/Thiolate IPC Model/RKS/90 degrees Constrained Optimization

C	30.80858667374381	-24.35999719293728	2.21033969720561
C	35.84548291906923	-24.84243258201186	10.77511095696186
C	39.01355278489130	-30.32739519648110	5.94416031957077
C	33.69197768014752	-28.40176383401482	0.29198324219816
N	33.22486881020414	-25.49747596715958	4.85062069563072
N	34.66004967644938	-25.63767771099560	7.30256283692321
N	34.80227164385145	-27.67635394572207	3.80408837906527
C	32.98450242934424	-26.52121012008587	2.63908842553168
C	32.91871901947556	-24.00451792326923	6.76542329000015
C	36.42705942169265	-26.84697691495545	8.49243773634597
C	36.68920145600812	-29.15977560101439	4.25939182201569
C	30.77424626127031	-22.65410377158107	4.98105846272373
C	33.50322588554167	-22.90651051233269	9.60572951541833
C	38.78747329711732	-28.81849596762766	8.82238577743956
C	36.20903036281643	-30.16088564253701	1.36532779167787
C	32.64538713008866	-25.59098732119228	3.61737626740145
C	33.87372886561116	-24.56377531237728	7.61128786452415
C	36.81169398018896	-27.72897703496642	7.48831179285858
C	35.68202847626870	-28.65448151221762	3.44429128101844
C	31.63044471086872	-24.55908457070865	3.44938197101536
C	34.17044401762612	-24.08136842145117	8.95311018905119
C	37.92604049405487	-28.66119314217243	7.60402265383279
C	35.42784258194568	-29.09787818594490	2.07923419287026
C	31.61734809493287	-23.83924916553431	4.61304007580782
C	35.15459896613454	-24.89565922238009	9.44446679183093
C	38.01898033782484	-29.29945197469511	6.39698434411785
C	34.37026748722727	-28.35991270075725	1.62869596813899
C	32.62275583624800	-24.44225200032101	5.47729347031531
C	35.44933516174667	-25.86160419622903	8.39472966251685
C	36.94910094913231	-28.76047456276606	5.56771766504815
C	33.99759943914852	-27.46944566074067	2.72145664388876
N	36.24083877086611	-27.81696305562392	6.25090428217565
Fe	34.66969644051564	-26.72025803788930	5.58467197387970
C	34.11166623502284	-31.37450134540431	7.28568917127088
C	35.36150570965706	-31.94940832591379	6.63878908734091
C	32.16113512914936	-27.54685853730795	6.92796640508291
C	33.45093878280928	-27.88972764214629	6.23134805492368
C	33.54497833186338	-29.37076132034278	6.11363321672314
O	33.12833032136894	-30.02784523531189	5.18506377815149
O	34.08775979384850	-29.9355660169547	7.23267930392249
H	30.057809335829141	-22.40786523855331	4.18944003305578
H	31.38463256900482	-21.75765845996602	5.15993909819032
H	30.19733065323448	-22.83340525152715	5.89919123152556
H	31.43491183974545	-24.11033673222745	1.34235553711986
H	30.24398456717211	-25.26459976975161	1.94441497215484
H	30.08436236803837	-23.54731018782700	2.33439774074837
H	33.74282276744074	-27.43136112296277	-0.22139489507972
H	34.15193969666664	-29.14479263826145	-0.36867264973263
H	32.62715495347405	-28.65839648851598	0.38355550300302
H	35.86052586610108	-30.29222464698869	0.33495877090622
H	37.27975349285030	-29.91813629898182	1.32001644431010
H	36.12380747416786	-31.13580084535075	1.86584927921147
H	33.90554252816626	-22.72132258329496	10.60788423598769
H	32.41908536180421	-23.05620374417854	9.71054533490974
H	33.64073703724409	-21.98567223474914	9.02180807171654
H	36.92904387366155	-24.69800007211053	10.66394649807605
H	35.70746847249750	-25.77158085844394	11.34608622150431
H	39.56120317277886	-29.57947421214611	8.67210175243908
H	39.29674516200105	-27.88072298883959	9.08480433763314
H	38.20068883919762	-29.11870764557700	9.70207009363495
H	38.52787345760246	-31.26965001515531	5.65339591273021
H	39.58276656577817	-29.97993575841011	5.07097016324632
H	39.73694340616183	-30.56364867770738	6.73268648801058
H	35.46679784948034	-24.02053924495806	11.39293162674909
H	36.25871592588960	-31.52461680894336	7.09372897970036
H	35.38255454932018	-33.03868300656868	6.76301364594627
H	35.37961013809958	-31.71882528758176	5.57294437753004

H	33.21060433793745	-31.76304544554661	6.80564328607610
H	34.07836125811233	-31.60765679042619	8.35302736105200
H	32.02298621503891	-26.47848774167507	7.06702110848573
H	31.31259035076496	-27.93762685490918	6.34575121796737
H	32.11716143992388	-28.04217222958743	7.90954372053957
H	32.43164823140244	-26.47457843001575	1.70542871774884
H	36.97688392777620	-26.89912854695286	9.42769555117040
H	37.33107263416798	-29.92710665162365	3.83706332916889
H	32.36374903793116	-23.14951131583751	7.14011524470383
S	36.41397614203375	-25.19217885329087	4.66582509066219
C	35.96546159285224	-23.44503406443325	5.00512763851088
H	35.00959934876124	-23.17201371908772	4.54278767770090
H	35.89167145480740	-23.24516768025043	6.08068259851616
H	36.74221440184661	-22.79085298796937	4.59017800205312

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B3LYP Scan/Thiolate IPC Model/RKS/100 degrees Constrained Optimization

C	30.80598905307545	-24.35138698557101	2.20581732984054
C	35.83242491587836	-24.88040399646430	10.77390033652359
C	39.00851917593812	-30.33754981050864	5.91766424335039
C	33.72294999943523	-28.35471685589768	0.25474253024009
N	33.22306374205243	-25.49950519852595	4.84076558381019
N	34.65370575259237	-25.65413371121205	7.29422095501504
N	34.80802488118780	-27.66647024571862	3.78235658431231
C	32.99206848925866	-26.50586199063711	2.62036465013756
C	32.91163147398309	-24.01933543036665	6.76480304470531
C	36.41826057398674	-26.87059944753363	8.48100316724666
C	36.69524489550705	-29.15162151228384	4.23179535938913
C	30.76222929563019	-22.66611333578156	4.98866352169294
C	33.49228383116819	-22.93728118428362	9.61197995486590
C	38.78393183695542	-28.83811143367691	8.80119925245561
C	36.23857614798149	-30.11808222448260	1.32459100189110
C	32.64611028836247	-25.58575705698287	3.60574844699206
C	33.86684948382685	-24.58206108572049	7.60805080529127
C	36.80465247820319	-27.74729860739036	7.47284957636458
C	35.69274555685078	-28.63775491656339	3.41690141313132
C	31.62739627511291	-24.55660751844616	3.44418532244525
C	34.16115252732591	-24.10772545053708	8.95323487086767
C	37.92083868911165	-28.67775529533308	7.58424801304356
C	35.44868964157137	-29.06622848319844	2.04527764326019
C	31.61035361964515	-23.84522662911499	4.61300749840971
C	35.14427395605240	-24.92505043462660	9.44153675613560
C	38.01570714096626	-29.30959117123949	6.37381165211616
C	34.39137690877318	-28.32704002061350	1.59674139731610
C	32.61702606875063	-24.45058341406830	5.47408469898631
C	35.44086026796823	-25.88470393547268	8.38664391515912
C	36.94705085152709	-28.76702963682591	5.54590558230630
C	34.00887922766146	-27.45060421351347	2.69766830498416
N	36.23468963371625	-27.82984664794311	6.23441274351676
Fe	34.66546898927776	-26.72639595420314	5.56899761806643
C	34.04797109433773	-31.36879533011431	7.34083246318125
C	35.35911138363331	-31.89734764420255	6.78029921023776
C	32.17929408006206	-27.55473193712098	6.94936668040207
C	33.44673270820384	-27.89776541895124	6.21321088315906
C	33.56069705772315	-29.37886663343342	6.10943769023496
O	33.28252137273860	-30.04905192217122	5.14016774257782
O	33.97344312600067	-29.93160105496950	7.29173197502160
H	30.04384734636431	-22.41872178774107	4.19917916214855
H	31.36863739469035	-21.76782322913548	5.17187038665961
H	30.18718601405296	-22.85321798374040	5.90640680878016
H	31.43019243744024	-24.07735729883343	1.34356418993284
H	30.25729432625226	-25.26085048434046	1.92394287608440
H	30.06793864587193	-23.55295744919497	2.34063760376412
H	33.77584354261186	-27.37844715641431	-0.24725835368127
H	34.18924302181090	-29.08928849146896	-0.41092558768178
H	32.65794360382557	-28.61442024266002	0.33514054305391
H	35.89769451494944	-30.23902173493232	0.29040053107852
H	37.30864251072986	-29.87082476654516	1.28935621453683

H	36.15339949317155	-31.09862058745226	1.81392770635537
H	33.89382394173096	-22.75719235414287	10.61537092396906
H	32.40827099707295	-23.08890021250388	9.71540524824016
H	33.62899436514193	-22.01308067652348	9.03324244343860
H	36.91650117060144	-24.73761606143869	10.66568651073205
H	35.69139112247083	-25.81237330261867	11.33952146841887
H	39.56190796723930	-29.59357952924996	8.64515979421543
H	39.28810422485794	-27.89905217303929	9.06873683421545
H	38.20027595443725	-29.14721424352193	9.67985164564331
H	38.52081866340728	-31.28053270971063	5.63255792981888
H	39.57210751423783	-29.99207916784506	5.04011777172249
H	39.73676474016309	-30.57153843528694	6.70234979211554
H	35.45420200576985	-24.06109682568022	11.39541498646240
H	36.20867098885298	-31.42652691334859	7.27946584346822
H	35.41958267915254	-32.98268127523951	6.92460255659151
H	35.43169987143128	-31.68210998001837	5.71383171805613
H	33.19673748090351	-31.78808719273984	6.79891930519372
H	33.94865325042642	-31.60781057813259	8.40268819242287
H	32.03010776908530	-26.48521937252275	7.06499507818589
H	31.30971313919149	-27.97263862721763	6.41821563509715
H	32.18860526228342	-28.02336180511766	7.94400483868966
H	32.44286235089039	-26.45226211825533	1.68493162082145
H	36.96690749747863	-26.92737019529913	9.41664508053337
H	37.34001350053862	-29.91378772882523	3.80461415602025
H	32.35472359933466	-23.16767925367071	7.14415736703123
S	36.41102106619646	-25.19161922631444	4.66318019067776
C	35.96202972887728	-23.44723601373980	5.01556992333198
H	35.00656898318953	-23.17121597719326	4.55420959026967
H	35.88690552648993	-23.25565875917304	6.09252499534986
H	36.73886197974139	-22.78961440347120	4.60628046555232

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B3LYP Scan/Thiolate IPC Model/RKS/110 degrees Constrained Optimization

C	30.80270897643953	-24.35943259708233	2.19733304450284
C	35.816649098866301	-24.89183881448590	10.77233348713866
C	39.00938751912339	-30.33779343000521	5.91629713445808
C	33.75684157527013	-28.33011722830660	0.23260586725475
N	33.22293172943313	-25.50168459940269	4.83161930232346
N	34.64632345200715	-25.66049840068407	7.28858207966213
N	34.82086249107392	-27.65665532964596	3.76949706869884
C	33.00198085083660	-26.50144904464744	2.60732896348713
C	32.90442281918248	-24.02605983458630	6.75831483237005
C	36.40606444123581	-26.88051193026120	8.47954590407285
C	36.71194556140300	-29.13691926145940	4.21935964058238
C	30.74858048687724	-22.68059031060856	4.98383241230148
C	33.48180276081943	-22.94485769743634	9.60635578397569
C	38.77112465192260	-28.84866794925480	8.80380156030273
C	36.27925506596738	-30.08297929456573	1.30365326168125
C	32.64807695696224	-25.58759485254503	3.59563294228355
C	33.85956321876160	-24.58799923612148	7.60182302469758
C	36.79740655731884	-27.75387457012941	7.47032573502748
C	35.71323675949488	-28.61979980087614	3.40218936002969
C	31.62428896111753	-24.56327994473676	3.43581040537377
C	34.15090499100727	-24.11543681648926	8.94810452632927
C	37.91359021717944	-28.68412427472874	7.58341934347488
C	35.47889027548643	-29.04075843820382	2.02662491356121
C	31.60274023326317	-23.85467819596735	4.60624640098541
C	35.13159263419540	-24.93465065541645	9.43830815534567
C	38.01546778582694	-29.31026481497243	6.37056535321962
C	34.41842438837170	-28.30639714321689	1.57800302159215
C	32.61151284155461	-24.45717389617090	5.46698779374882
C	35.42994541534378	-25.89340490983271	8.38311463482418
C	36.95230681372340	-28.76358232825466	5.53861273400922
C	34.02508416036973	-27.43957050890602	2.68291108317233
N	36.23411737883153	-27.83132718842011	6.22829905787308
Fe	34.66496412197446	-26.72743948393570	5.55893908883672
C	33.96246677457817	-31.39294624496402	7.31823730775185
C	35.32508986917541	-31.88292276109740	6.85204875955188

C	32.22290650010945	-27.55973039280374	7.00429891521170
C	33.44894283311852	-27.90411453208471	6.20137139951075
C	33.56784447523227	-29.38405303298099	6.08231289291430
O	33.40762895302262	-30.04309118517728	5.08006727813581
O	33.85935415475769	-29.95742978741026	7.29447813694484
H	30.02961282805600	-22.43498510751380	4.19431561088612
H	31.35040727238316	-21.77968807292561	5.16940241135936
H	30.17374388080326	-22.87241875655225	5.90072477468329
H	31.42579559400190	-24.07823390637688	1.33656269499705
H	30.26050571210137	-25.27166401557610	1.91190732717046
H	30.05909164060890	-23.56651334038015	2.33408873344254
H	33.80493854887668	-27.35023482983494	-0.26283152268306
H	34.23203676110294	-29.05675677295217	-0.43548519806404
H	32.69344072068692	-28.59850421899603	0.30573436467080
H	35.94580445986687	-30.19866788827254	0.26643590676150
H	37.34809985880544	-29.82950428228151	1.27713601026278
H	36.19625557105110	-31.06718772725137	1.78593699806909
H	33.88117287114552	-22.76608407007054	10.61084719754034
H	32.39739499132885	-23.09541424072916	9.70714563081441
H	33.62083521977794	-22.02032076023895	9.02873704732696
H	36.90091352226985	-24.74836964559395	10.66681655559490
H	35.67482151017850	-25.82473677217346	11.33620909118461
H	39.54891125080705	-29.60459700212355	8.64908695886390
H	39.27537189934861	-27.91085724888563	9.07568905636245
H	38.18372585070546	-29.15916253954280	9.67943403549625
H	38.52170714640701	-31.27899142268398	5.62550032849815
H	39.57809366052944	-29.99032194705171	5.04283233754881
H	39.73318410377905	-30.57547437620238	6.70396386507602
H	35.43665678496406	-24.07368348292642	11.39428133493061
H	36.12406729520355	-31.40323396768398	7.42152357974858
H	35.39995018606675	-32.96898909848736	6.98347797013961
H	35.47268894356512	-31.64738831540144	5.79801136289950
H	33.16680286157506	-31.81725410509845	6.70072430569095
H	33.78355439659653	-31.65887100981603	8.36314629815347
H	32.02724279198975	-26.49213049751741	7.04123145161322
H	31.33089006508257	-28.06801549854594	6.60609491399440
H	32.35421791553657	-27.92931023174440	8.03118796752970
H	32.45501509771845	-26.44689631562507	1.67062732154564
H	36.95065448252694	-26.93992638477660	9.41738109701162
H	37.36168643516689	-29.89395648040729	3.79061027194290
H	32.34521992135267	-23.17606026179142	7.13797182308356
S	36.40611024936936	-25.18489513921551	4.65987468125351
C	35.96269082751338	-23.44380637475090	5.03391941975350
H	35.00536254890248	-23.16144852460132	4.58027972684531
H	35.89306497138929	-23.26391532580846	6.11323567794257
H	36.73851728482558	-22.78310942371670	4.62775237884045

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B3LYP Scan/Thiolate IPC Model/RKS/120 degrees Constrained Optimization

C	30.79103516330960	-24.35339396071719	2.20333450424743
C	35.82194203990168	-24.93184452475671	10.76481908993206
C	39.02854881822228	-30.32742363257515	5.86580246456383
C	33.77908205271014	-28.27724166139684	0.19402561771559
N	33.22075468006625	-25.50634925833851	4.82436333088210
N	34.64423640108028	-25.68277265320955	7.27963137481247
N	34.83190329258702	-27.63962572924568	3.74082969432014
C	33.00343808568498	-26.48677394930380	2.59130036872632
C	32.90103447426394	-24.04540504432058	6.76209117438022
C	36.40591099335118	-26.90937337618414	8.46116399192611
C	36.73266176949744	-29.11233099851057	4.17476658500191
C	30.73761876668098	-22.69445532788727	5.00141447708807
C	33.48528419801380	-22.97853965069977	9.61328998654759
C	38.77797799537574	-28.87137247900318	8.76813974304479
C	36.31742342763556	-30.01875837308568	1.24619760413503
C	32.64448009769197	-25.58465006260617	3.58843683024345
C	33.85790581364719	-24.61209524161826	7.60026503334172
C	36.79998699225508	-27.77314671123586	7.44444794718795
C	35.73367528742743	-28.58936823602216	3.36249936052507

C	31.61620643617523	-24.56344452368244	3.43839795475549
C	34.15192604070837	-24.14676612184698	8.94836963969017
C	37.92097547348695	-28.69839795522363	7.54847145408694
C	35.50560896076674	-28.99406935630490	1.98119864062270
C	31.59466163424545	-23.86323677030858	4.61395441848173
C	35.13314905770875	-24.96891135134922	9.43254366040031
C	38.02793084716538	-29.31039043709310	6.32891429517621
C	34.43800827159186	-28.26516364081362	1.54085405523910
C	32.60703830740543	-24.46840839476975	5.46835315443602
C	35.42935867557569	-25.92216443354734	8.37180955080552
C	36.96414191319786	-28.75940850913822	5.50088376399571
C	34.03503353339133	-27.41658189950010	2.65653242419093
N	36.23798852198394	-27.84054373991911	6.20102639627304
Fe	34.66568952648195	-26.73511485767649	5.54074262382778
C	33.84438172238364	-31.40852536022178	7.35071787806801
C	35.28669695871133	-31.85344796081809	7.15970907533172
C	32.22749617147079	-27.57717862587463	6.97759913982295
C	33.45207921002387	-27.92249438469987	6.17235900983934
C	33.59811518459815	-29.40226874611977	6.06723113585002
O	33.61251038708556	-30.06752048075738	5.05697372491387
O	33.70942028338257	-29.97753159732933	7.31408180800958
H	30.01526519944701	-22.44668697838932	4.21568579096129
H	31.33700620546696	-21.79256466684700	5.19015835671538
H	30.16651247101108	-22.89349928543394	5.91907986076470
H	31.40952307160242	-24.05397250083789	1.34533776259935
H	30.25898610747992	-25.26809247802208	1.90705669508784
H	30.03843189757023	-23.57096347008365	2.35105760824110
H	33.82098582464923	-27.29113423037429	-0.28957118851501
H	34.26093158858718	-28.99220964324588	-0.48185557906824
H	32.71749444606997	-28.55433889594636	0.26139106578201
H	35.98750132434842	-30.12374023390626	0.20670215144795
H	37.38381391196637	-29.75471489090556	1.22571652093667
H	36.24245792900236	-31.00976737591337	1.71555476367257
H	33.88826615749005	-22.80330662400338	10.61696290371188
H	32.40121518465364	-23.12926496943557	9.71740892407916
H	33.62243819905254	-22.05200483165282	9.03843791305694
H	36.90609191076037	-24.78961670047529	10.65651794855796
H	35.68038520638884	-25.86634198086564	11.32608333451824
H	39.55924484068300	-29.62226450207774	8.60672162566264
H	39.27791596856132	-27.93408070640860	9.04975698904391
H	38.19143044986491	-29.19295783972830	9.64039344430266
H	38.54820037231544	-31.26994096167539	5.56736951085064
H	39.59427574881852	-29.96855231251763	4.99503761427149
H	39.75432508665796	-30.56623151538354	6.65121959182807
H	35.44509267651712	-24.11511146136809	11.39056167600801
H	35.94213173159209	-31.37143450634135	7.88860756904865
H	35.36650288702651	-32.94046294368577	7.27932828336720
H	35.63748085865840	-31.58630185248910	6.16252453533698
H	33.20029082317648	-31.84738520015906	6.58509163751242
H	33.47006012041085	-31.69308713211959	8.33773952521203
H	32.01704303655611	-26.51195512830116	6.98867171010655
H	31.33713985208679	-28.10781948163116	6.60560540920512
H	32.37503229048490	-27.91754921683520	8.01157570431881
H	32.45580018801973	-26.42662207400984	1.65532734964734
H	36.95113139622180	-26.97464984301511	9.39822197072424
H	37.38814789909795	-29.85926669572775	3.73724805723820
H	32.34113602606037	-23.19887611756753	7.14836660117385
S	36.40117446944317	-25.17676691322494	4.65688836203447
C	35.94791204807640	-23.43942147164190	5.03568056662644
H	34.99001288442578	-23.16110813754410	4.58072433536839
H	35.87450248911161	-23.26363522460892	6.11542646520385
H	36.72087843864168	-22.77308908788886	4.63335805691908

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B3LYP Scan/Thiolate IPC Model/RKS/130 degrees Constrained Optimization

C	30.58800810312517	-24.34082425471636	2.21889180035137
C	35.52908844528531	-25.04057159011938	10.82264339582801
C	39.11086313406791	-30.00992115715408	5.71764956861134

C	33.81896634587823	-27.99481731198866	0.07627797666452
N	33.05867402678308	-25.46539434027681	4.81411232646711
N	34.47653215254120	-25.65793671703632	7.27256292540421
N	34.81865199798231	-27.42853280217646	3.65084498375348
C	32.91471148459246	-26.35998545269281	2.54089063473783
C	32.65794711333534	-24.09297069530540	6.79904600960765
C	36.28175381678542	-26.84703220350311	8.42647553732041
C	36.80196008963624	-28.80505393935108	4.03935854599348
C	30.44464633734205	-22.78242584164420	5.07140629438792
C	33.11920187875077	-23.15388484977614	9.71678917789170
C	38.73537612556670	-28.72147824439433	8.68601101234739
C	36.45923645069156	-29.61161045641457	1.07383965276900
C	32.49661102767178	-25.52437082691082	3.57117414411137
C	33.62760530242822	-24.65053204738043	7.62842020152304
C	36.74632095629498	-27.63017029739809	7.37266691934000
C	35.78064246395549	-28.30629344313220	3.24095628634888
C	31.41708548607829	-24.55233961106113	3.45103209559242
C	33.86588050070622	-24.24423485403950	9.00650906473845
C	37.90278924827913	-28.51212709508025	7.45514039846341
C	35.58280270796730	-28.66902462880376	1.84411471915384
C	31.35704606487798	-23.89571104880727	4.64933462764027
C	34.87860872711876	-25.03792811651364	9.47121424748257
C	38.06361634431847	-29.05353079454670	6.20724766276501
C	34.46994804854184	-27.99390481289257	1.42725486678627
C	32.39413735511245	-24.48092675350889	5.48844826967026
C	35.25271803468009	-25.91277326133767	8.36773642760920
C	36.99818557236954	-28.50257878143023	5.38260817340981
C	34.00910928395350	-27.21851571555462	2.57250607149026
N	36.21786087230341	-27.65179514290722	6.11243661003040
Fe	34.58080548926301	-26.62410107436515	5.48623326884965
C	34.38074143685571	-31.17273909467146	7.52207405652434
C	34.53390909101641	-31.44024522124142	9.00796598053740
C	32.17740638166173	-27.66469784976236	6.85511459493697
C	33.45299600856846	-27.90652844409551	6.09401892659861
C	33.81615154769148	-29.35165496027922	6.09140945526786
O	34.11305901121852	-30.04676759594440	5.14788097192866
O	33.84359370364388	-29.85127989859680	7.37753876843390
H	29.70645152258725	-22.55038035947210	4.29559107616711
H	31.00050736735206	-21.85765872692527	5.28081945972343
H	29.88953265800255	-23.03325398750048	5.98617986002982
H	31.19045500449844	-23.95961351402255	1.38212391884244
H	30.12150274189471	-25.27454178854144	1.87507529255701
H	29.78267881904728	-23.61920965095801	2.39552660625880
H	33.78692950556378	-26.98702111841169	-0.36092046742981
H	34.35737875470568	-28.63847495185663	-0.62804841826089
H	32.78158657495400	-28.35540952934909	0.12194823333009
H	36.14691276267499	-29.68646680170519	0.02632552426690
H	37.50937850709482	-29.28836841454882	1.07970405995767
H	36.43500268183000	-30.62583635147068	1.49652054341296
H	33.45832884918446	-23.04209369939606	10.75260696744217
H	32.03811111616885	-23.35053938159308	9.74619010990167
H	33.25152966919783	-22.18181758315448	9.22168270754089
H	36.59912626580881	-24.79837034248825	10.75911773523528
H	35.45437667830375	-26.02254993260233	11.31112311834134
H	39.55151241498947	-29.42929022550874	8.50354271449044
H	39.18804648906174	-27.78303135515964	9.03554424632416
H	38.14108061715978	-29.11678734389003	9.52203600412728
H	38.66733845718905	-30.94038492744938	5.33672653249552
H	39.69957088933921	-29.57882745512639	4.89594479496918
H	39.81237407075734	-30.28382946787540	6.51354377996353
H	35.06714957927805	-24.30726953389154	11.49287810427367
H	33.56926211717702	-31.37897896793122	9.51970819041218
H	34.95006313100681	-32.43917728739158	9.17700773884497
H	35.20411800473273	-30.70450001033850	9.45911973174327
H	35.33971340125066	-31.22852888676649	7.00064795090098
H	33.70852821382068	-31.89521951338462	7.04633297754173
H	31.84923306286385	-26.63070390907616	6.80840209320284
H	31.36251191495898	-28.30764095120568	6.48743829358249

H	32.32877270020970	-27.93869553186643	7.90743527192672
H	32.36755225589017	-26.29676429640770	1.60484918104970
H	36.80922115501460	-26.93572080708983	9.37180735175011
H	37.49578574649538	-29.50277907991046	3.58028600043092
H	32.05315630467360	-23.29144212000093	7.21246004258674
S	36.04099761314997	-24.71622045256434	4.80515613430323
C	37.51389534426846	-25.33141204263112	3.90086758138025
H	38.12630476768874	-25.99548597811653	4.52236599825743
H	37.23320628767631	-25.87957790759033	2.99386404049693
H	38.13305449853730	-24.47619468801911	3.60334667226059

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B3LYP Scan/Thiolate IPC Model/RKS/140 degrees Constrained Optimization

C	30.62077274599416	-24.38188628377292	2.21232521579366
C	35.45713462120580	-24.95946224542272	10.88395583599195
C	39.12306219777866	-29.96766021260016	5.88674922454586
C	33.86928102969253	-28.07731312803699	0.16613753326260
N	33.06503408205938	-25.46343918463812	4.85032200583490
N	34.44741875127964	-25.62647971782233	7.33036928805209
N	34.82787156837992	-27.45484343764666	3.74279365991111
C	32.93551925434494	-26.40523769889336	2.59549948393221
C	32.65476586163506	-24.04870004141305	6.80345997153447
C	36.22884677535845	-26.80832770609019	8.52762699903047
C	36.81428484366609	-28.81404574224536	4.17084618288907
C	30.46623522624161	-22.75999660786458	5.02825612164749
C	33.08539103479801	-23.06490602805660	9.71184343272984
C	38.69902169589309	-28.65076453181394	8.83553113680764
C	36.51171691713846	-29.65865718409301	1.21193053109758
C	32.51240642054729	-25.54662596471629	3.60444475172440
C	33.60628056746597	-24.60219731896905	7.65610731486320
C	36.70856590650353	-27.60315017114504	7.48972103050079
C	35.80005488175970	-28.33090831015470	3.35448673169956
C	31.43993520700663	-24.57096668810804	3.45471816136234
C	33.82916130176622	-24.17541004496605	9.03042852750597
C	37.87532242613071	-28.46885191703225	7.59445644900632
C	35.62000217618851	-28.71304266141141	1.96072424498405
C	31.37544200678650	-23.88716252386746	4.63751502659870
C	34.82516726283418	-24.97313466713708	9.52377129126020
C	38.05565774020221	-29.02271340399947	6.35508188169429
C	34.50628538668089	-28.05231688055549	1.52351710634094
C	32.40168026701500	-24.46046671812513	5.49794829095842
C	35.20540482233680	-25.87033092513008	8.44077275525346
C	36.99007232657240	-28.49656190430629	5.51354346720101
C	34.02935273731663	-27.26351947316299	2.65307133991452
N	36.19297592119083	-27.64597068606794	6.22482693233351
Fe	34.56763522746385	-26.62446010573058	5.56368083870571
C	33.75809667160044	-31.33575821018940	7.45703513065380
C	35.22735068923135	-31.55156624014674	7.79193109853162
C	32.14869267816268	-27.58734377053744	6.93838223964045
C	33.40544708766657	-27.88577160469499	6.16274217074338
C	33.68157534324504	-29.34993584304872	6.11543606068132
O	34.09191640276673	-30.00380074536609	5.18426086096364
O	33.43903294886126	-29.94122194965422	7.34505202543262
H	29.73788108604986	-22.53765908618409	4.24034834651142
H	31.02593178655261	-21.83511855382985	5.22652398141410
H	29.89960892609742	-22.99013934930501	5.94141538315386
H	31.23101992850057	-24.02250639606279	1.37153855312552
H	30.15101817782785	-25.32019793313561	1.88589119554440
H	29.81870393959942	-23.65179273394239	2.3676063261217
H	33.83382857816844	-27.07626900824295	-0.28606271519922
H	34.42013492285959	-28.72661368271264	-0.52326222229255
H	32.83445061079989	-28.44581941086873	0.20616376319865
H	36.21576450411915	-29.74361522803136	0.16042614157133
H	37.56021033212667	-29.33071789927161	1.23078940837298
H	36.48553365051430	-30.66945564837380	1.64267006027821
H	33.41480278187009	-22.93678669524350	10.74890857805958
H	32.00229819427815	-23.25118035997791	9.73334833164987
H	33.23212164683738	-22.10370861352136	9.19993859004779

H	36.52947548341798	-24.72479687952660	10.83138764214923
H	35.36980073488327	-25.93360812054936	11.38569652035200
H	39.52324166287165	-29.35347491916450	8.67082597974538
H	39.13927316076310	-27.70257089321035	9.17449542468584
H	38.10089461120730	-29.03955219652116	9.67170271839704
H	38.69969190469240	-30.91170790328794	5.51655571799511
H	39.71013602067970	-29.53775115474605	5.06327252714034
H	39.822330316844972	-30.21773862897732	6.69156959076921
H	34.99089476057851	-24.21345590348210	11.53692615994393
H	35.49868962443185	-31.01500586649722	8.70480471189115
H	35.43218889363600	-32.61836535286558	7.94070108960494
H	35.86119003063091	-31.18529605264729	6.98351307736786
H	33.49567439485839	-31.84085600430700	6.52488841805698
H	33.11183825852251	-31.70528828282689	8.25805310021646
H	31.82825319515906	-26.55565968328895	6.83242956765563
H	31.31785964644945	-28.24807271419643	6.65078643302843
H	32.33393535352275	-27.78206767694664	8.00287793404992
H	32.39704327496442	-26.35907823771834	1.65346646492757
H	36.74372139211285	-26.88504041636804	9.48086366045686
H	37.52129508278449	-29.50910429315098	3.72804548780649
H	32.05322908581020	-23.23334050360350	7.19387277649362
S	36.04980304382117	-24.73701657752811	4.87058467850254
C	37.51452687299260	-25.36185593189774	3.96060506622020
H	38.12647160944758	-26.02724629120875	4.58123274640877
H	37.22563526219808	-25.91196850916335	3.05741380156265
H	38.13624007714382	-24.51087202898254	3.65659703090859

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B3LYP Scan/Thiolate IPC Model/RKS/150 degrees Constrained Optimization

C	30.58978831400419	-24.42211185439041	2.22759752974838
C	35.46547248173027	-24.99683824053750	10.87532825773105
C	39.16965396206390	-29.92930807232990	5.82779756415937
C	33.86905281823238	-28.06953187711382	0.14676313114740
N	33.07324638499231	-25.47328637984475	4.84095408143667
N	34.47076265825123	-25.63071150923609	7.31189936591649
N	34.85136259715077	-27.43734622883954	3.71559959327722
C	32.92919523144817	-26.41972483176780	2.58905467375283
C	32.66708180181065	-24.06170754148380	6.79738954870672
C	36.25182954093300	-26.81954074384613	8.50224288864240
C	36.87092873844556	-28.75395463629727	4.11842351071020
C	30.45460092537896	-22.79034911854498	5.03949187102515
C	33.09104106455310	-23.09879763144921	9.71412829050652
C	38.71817428402082	-28.67027906894400	8.79934199545490
C	36.56145898078832	-29.58877360225300	1.15727845621280
C	32.50738205117938	-25.56470023423184	3.60163296088725
C	33.62352288580739	-24.61387189886107	7.64510158361666
C	36.73954359761458	-27.59759852596131	7.45534545399686
C	35.84122626179201	-28.28722133037743	3.31275624411633
C	31.42487911767042	-24.59916150167540	3.46117127813339
C	33.84180586952657	-24.19896769398275	9.02367638091813
C	37.90626659159538	-28.46497852899083	7.55426034466185
C	35.65583218546384	-28.66711212854100	1.91926169783030
C	31.36867360935301	-23.91128715085387	4.64221228851751
C	34.83888141016670	-24.99830904619409	9.51261577461882
C	38.09859105371464	-28.99347577092734	6.30562114123619
C	34.52086579275399	-28.03292363876935	1.49693769004969
C	32.40841302940124	-24.47378163461178	5.49312313878266
C	35.22617418128037	-25.88305609723141	8.42210796099836
C	37.03877220134515	-28.45369961786921	5.46553546433433
C	34.03805692413648	-27.25911662129462	2.63421140335197
N	36.23372222952911	-27.61954429509866	6.18619772769168
Fe	34.59422650436574	-26.61824365731016	5.54164636064304
C	33.63627038655734	-31.36903141254448	7.43960632226538
C	34.98363788469265	-31.55596024309881	8.12405589279824
C	32.18662307670365	-27.59547992657694	6.91838222665838
C	33.45170496913701	-27.89611733120337	6.15668398137180
C	33.75651137542115	-29.35486251030186	6.13690350525709
O	34.33464458192012	-29.98744473843670	5.28282115548024

O	33.1237331589028	-29.98034085098263	7.29625274526552
H	29.71926989631132	-22.57295561834051	4.25672320306151
H	31.00963194296670	-21.86187141850315	5.23380502205110
H	29.89593114078880	-23.02420762140503	5.95660409907232
H	31.18818677299838	-24.06583494285583	1.37706209285606
H	30.12037258727213	-25.36474631405751	1.91327190352697
H	29.78630750837148	-23.69462830702604	2.38768784597521
H	33.80154441685379	-27.06798145642472	-0.30049237145782
H	34.42928919414035	-28.70089522836588	-0.55171342515406
H	32.84492118572498	-28.46579718019944	0.19673815671005
H	36.25325103867716	-29.68095557267017	0.10991705798432
H	37.60127831673890	-29.23380930212096	1.16231396415724
H	36.56742694799733	-30.60005071745459	1.58766218452634
H	33.41582341768970	-22.98074464892114	10.75384073220317
H	32.00868768058554	-23.28970916576842	9.72931647757916
H	33.23591178696593	-22.13149912252200	9.21332546617315
H	36.53737516245319	-24.75877098420880	10.82956352790866
H	35.37871886536540	-25.97631379440031	11.36674317995733
H	39.54272701105732	-29.37156388025743	8.62998802398864
H	39.15712075721160	-27.72909532373199	9.15903786633350
H	38.11098651530427	-29.07253438199526	9.62239835607522
H	38.74719868968908	-30.86221500791718	5.42989310025450
H	39.76782432633976	-29.48133258281281	5.02202584817546
H	39.85944715451072	-30.20062273396571	6.63475607270297
H	34.99457159460953	-24.25888670977973	11.53406180604837
H	34.99602239513331	-31.04960629883050	9.09314151879958
H	35.18752153036399	-32.62094363615363	8.28615841462420
H	35.78629839060752	-31.13990200085004	7.51258862081519
H	33.63231473423801	-31.84349932734959	6.45638062701570
H	32.82688822626973	-31.78869961347951	8.04413419457974
H	31.83854775129830	-26.57975270385039	6.76006548429188
H	31.37568409800871	-28.29385005958500	6.67013242240411
H	32.37533233303446	-27.72511769496749	7.99253261350242
H	32.37987757715255	-26.38174135872222	1.65294303314673
H	36.76158914429125	-26.90836015206221	9.45717322530757
H	37.58834565025524	-29.43263269956163	3.66711828569977
H	32.06170236524054	-23.25179160759828	7.19310361964640
S	36.04540036804503	-24.70722600679421	4.85002219386855
C	37.52770130584562	-25.30279130997365	3.94973998211018
H	38.14256813312458	-25.96440968549853	4.57147217055225
H	37.25561767388734	-25.85062791698437	3.03985255259663
H	38.14002022675825	-24.44075828922836	3.65821377441985

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B3LYP Scan/Thiolate IPC Model/RKS/160 degrees Constrained Optimization

C	30.56161155438959	-24.49362592103346	2.26609921828333
C	35.50465097559162	-24.94972566009353	10.88151136743793
C	39.25065233516479	-29.84362603659985	5.83191066395053
C	33.86622654173403	-28.12096095041770	0.18956839661883
N	33.08353080284984	-25.48793355322409	4.86460601202601
N	34.49993881523788	-25.61150134399660	7.32621670107297
N	34.87827857546451	-27.43561221969695	3.74013934136828
C	32.92326590752958	-26.46554450920684	2.62744530725575
C	32.68816565047324	-24.05349393031083	6.80658083690506
C	36.29149366416316	-26.78336490642481	8.51623139418511
C	36.93559956026687	-28.69712131713424	4.12756291405076
C	30.45089197193154	-22.81855016344930	5.05365727909122
C	33.12378063980742	-23.06398455260067	9.71370653527625
C	38.77562744657877	-28.60980800072178	8.81051016858144
C	36.61305883262333	-29.55765956759014	1.17408443384909
C	32.50339859466081	-25.60224336380949	3.63378584729823
C	33.65143887155344	-24.59403010019305	7.65442006079601
C	36.78626831547260	-27.55500261670695	7.46799395785112
C	35.88589816126031	-28.26163494184478	3.33035414084140
C	31.41254059958971	-24.64642496031577	3.49211980763129
C	33.87371350258929	-24.16827034654837	9.02896266521486
C	37.96561439838306	-28.40614618233296	7.56402610189581
C	35.69310779033631	-28.65511964679142	1.94188653398759

C	31.36692144259443	-23.94012885869499	4.66281518866371
C	34.87342691398410	-24.96260119735432	9.52096090031809
C	38.16825101939980	-28.92296451590977	6.31279137123264
C	34.53556307146589	-28.05497697951971	1.53012818083896
C	32.41979304439448	-24.48333609455632	5.50994790996694
C	35.25972991357117	-25.85371498723121	8.43553794352581
C	37.10036600826131	-28.39605753547232	5.47461862578847
C	34.04793565707281	-27.28450720834356	2.66745847037072
N	36.28168841487225	-27.57875891112259	6.19893541565642
Fe	34.62444243292182	-26.60913263136724	5.56198372807695
C	33.41260108036237	-31.45444596416733	7.25110047443300
C	34.68794527375822	-31.74080770089050	8.03372791086747
C	32.23061280563958	-27.59445180724602	6.94884593905637
C	33.49612126087348	-27.89847913239477	6.18970901731067
C	33.78825366543121	-29.35910281457567	6.14549085239278
O	34.50317122890310	-29.95712552327260	5.37226424438542
O	33.14311267453552	-30.05058687959973	7.16811174143659
H	29.70932268517956	-22.61294852068614	4.27359096487619
H	31.00351377779747	-21.88579687717165	5.23365946725415
H	29.89939276389847	-23.04417233817288	5.97717474266269
H	31.14863096706375	-24.15224814734336	1.40165210320672
H	30.08987378465779	-25.44261124980578	1.97511884836044
H	29.75895621687928	-23.76449049647570	2.42277934459547
H	33.75874843674209	-27.12484147610813	-0.26183838093878
H	34.43742252064598	-28.73710742009176	-0.51364639277164
H	32.85667116990918	-28.55089899376405	0.25611041736283
H	36.28864269022212	-29.67257897843988	0.13389149684909
H	37.64122334793083	-29.17046284851607	1.15566565227915
H	36.65866722380083	-30.56271951227930	1.61640769132353
H	33.45428629064821	-22.93560133963507	10.75039038622802
H	32.04204294881715	-23.25761668289407	9.73687704472281
H	33.26323759273624	-22.10094769619307	9.20325523926937
H	36.57536592200339	-24.70732688623582	10.83066457521249
H	35.42381896066744	-25.92646244777286	11.37933376193727
H	39.60728339908579	-29.30247267881577	8.64033817832398
H	39.20460391918267	-27.66645058446730	9.17666304310731
H	38.16925094112495	-29.02173477655044	9.62939772673667
H	38.83864654709416	-30.77988937509365	5.43094226445767
H	39.84346450235582	-29.38586832317016	5.02761983379914
H	39.94370858038145	-30.10952860759258	6.63789365663015
H	35.03274851152874	-24.20976393074526	11.53726156605059
H	34.63649730418830	-31.29612103303619	9.03165983173432
H	34.83607020941838	-32.82152394318729	8.14349698215796
H	35.55354957843360	-31.32467213450997	7.51608961505451
H	33.48020124341144	-31.87044071465075	6.24334268391270
H	32.53947385840905	-31.87867217235264	7.75523510061170
H	31.92578708246772	-26.55816741206608	6.85095266369795
H	31.39989412804304	-28.23987800432127	6.63305070551038
H	32.38075002894248	-27.80663437454264	8.01608212974472
H	32.36226899929223	-26.44706095915373	1.69768072714971
H	36.80330235495079	-26.86718517799633	9.47053133227170
H	37.66687361616812	-29.35816147106252	3.67229094340737
H	32.08239055450689	-23.24158325479683	7.19755086694501
S	36.04599844593950	-24.68032246911660	4.85814100154050
C	37.50877616978287	-25.24934584246702	3.91108115382016
H	38.14354062084946	-25.91608995278855	4.50672279469724
H	37.21691333302451	-25.78601522338485	3.00055985545265
H	38.10698604112438	-24.37830223978327	3.61723518696605

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B3LYP Scan/Thiolate IPC Model/RKS/170 degrees Constrained Optimization

C	30.534565	-24.573760	2.313193
C	35.563232	-24.867051	10.885589
C	39.335249	-29.751603	5.852757
C	33.849227	-28.206149	0.258158
N	33.093187	-25.504937	4.899151
N	34.533346	-25.583272	7.347969
N	34.905848	-27.438298	3.778474

C	32.917034	-26.520728	2.680433
C	32.708701	-24.042251	6.821655
C	36.342523	-26.726572	8.537062
C	36.997278	-28.646421	4.153023
C	30.444703	-22.850805	5.072116
C	33.168232	-23.004874	9.708767
C	38.845405	-28.524753	8.831418
C	36.647045	-29.559788	1.216550
C	32.499596	-25.645459	3.677414
C	33.683300	-24.564371	7.668369
C	36.841787	-27.496631	7.490015
C	35.926606	-28.246528	3.364668
C	31.399906	-24.700342	3.532209
C	33.915044	-24.117906	9.034752
C	38.034286	-28.329603	7.584353
C	35.720506	-28.664963	1.985576
C	31.362968	-23.973893	4.690919
C	34.921016	-24.902023	9.530487
C	38.243026	-28.842754	6.333242
C	34.542123	-28.098567	1.584133
C	32.428834	-24.495280	5.535397
C	35.302707	-25.806272	8.454520
C	37.164281	-28.334863	5.497154
C	34.055965	-27.320635	2.716884
N	36.333723	-27.530720	6.223010
Fe	34.657566	-26.597370	5.594016
C	33.202123	-31.529069	6.953891
C	34.350031	-31.950072	7.863574
C	32.288225	-27.599610	7.005458
C	33.546482	-27.899503	6.233193
C	33.815951	-29.361259	6.133828
O	34.641458	-29.925606	5.449251
O	32.993328	-30.113325	6.972357
H	29.699509	-22.656535	4.292595
H	30.995274	-21.914461	5.239044
H	29.897351	-23.067195	6.000344
H	31.112807	-24.257410	1.433513
H	30.054140	-25.527047	2.051695
H	29.737835	-23.836399	2.461277
H	33.692350	-27.220350	-0.201143
H	34.430503	-28.806750	-0.450262
H	32.859299	-28.675457	0.349974
H	36.305875	-29.701290	0.185012
H	37.665387	-29.149445	1.171780
H	36.724345	-30.555212	1.675895
H	33.511283	-22.856023	10.738614
H	32.087698	-23.202556	9.749103
H	33.297155	-22.050925	9.178852
H	36.632605	-24.621685	10.822590
H	35.489884	-25.836752	11.398098
H	39.684751	-29.208211	8.661851
H	39.263383	-27.577077	9.199222
H	38.242127	-28.943951	9.648991
H	38.933365	-30.696465	5.461613
H	39.916956	-29.292052	5.041426
H	40.036628	-30.001861	6.656579
H	35.093740	-24.119359	11.534265
H	34.182191	-31.601043	8.886541
H	34.442152	-33.042385	7.883016
H	35.290831	-31.530638	7.504490
H	33.390729	-31.853189	5.927747
H	32.254583	-31.955844	7.295054
H	32.032155	-26.546115	6.993185
H	31.435215	-28.173420	6.618949
H	32.401878	-27.914622	8.051906
H	32.343153	-26.525833	1.758348
H	36.860379	-26.798617	9.489082
H	37.739069	-29.294505	3.696089

H	32.101955	-23.227881	7.205977
S	36.048090	-24.651828	4.872067
C	37.483152	-25.201701	3.873198
H	38.142417	-25.866040	4.444311
H	37.165057	-25.737120	2.970717
H	38.063820	-24.324141	3.564126

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B3LYP Scan/Thiolate IPC Model/RKS/180 degrees Constrained Optimization

C	30.49046798446964	-24.70688532407508	2.39444119148319
C	35.66256980178952	-24.74958074956819	10.88600721919266
C	39.45880007374706	-29.63096589664518	5.87379269368490
C	33.83561193743628	-28.32087454205186	0.35355065389144
N	33.11417177471492	-25.53490323906788	4.95004107779474
N	34.59411444929718	-25.54401725531054	7.37682064987044
N	34.94301987105899	-27.45691065771419	3.83579612068498
C	32.91583377595857	-26.60141387141548	2.75694575838756
C	32.73814349203140	-24.04065097586512	6.84939676400311
C	36.43794416299765	-26.63679201297919	8.55833757978217
C	37.06739475867438	-28.61135167853519	4.19548374763800
C	30.42121818392727	-22.92645344394537	5.11727700861616
C	33.22636478068792	-22.94123362302497	9.70980590658879
C	38.97993794807683	-28.37801609323512	8.84260613177644
C	36.68051262334509	-29.59324956559409	1.28356518515918
C	32.50036316922431	-25.71282515955242	3.74297665784692
C	33.73454391150484	-24.53067374695767	7.69041024013168
C	36.93603594131245	-27.41299755268891	7.51558692340306
C	35.97274250235635	-28.25246908188934	3.41929285089572
C	31.38122113670769	-24.79088245897559	3.59887524103369
C	33.97882101725300	-24.05613306348920	9.04532049779696
C	38.14917665275703	-28.21652495478050	7.60377017786912
C	35.74995241558196	-28.70288238757113	2.05301014783362
C	31.35306390457076	-24.04036671756458	4.74255379942340
C	35.00230221506259	-24.81738105553405	9.54086214831750
C	38.35243086023858	-28.74115225754416	6.35717453695845
C	34.55217564546169	-28.16948900792393	1.66269894569963
C	32.44325190865062	-24.52477682470408	5.57791041296130
C	35.38182783023183	-25.73539288887209	8.47580921329567
C	37.24891559300540	-28.27223673228422	5.53053521202134
C	34.07096509784883	-27.37852448974950	2.78817651127821
N	36.41018881401016	-27.47719028206191	6.25746443881549
Fe	34.70841376764346	-26.58676777052320	5.63790842883115
C	32.92958308313113	-31.54133762336263	6.53305859944326
C	33.80634889927468	-32.16528371130490	7.61205596443301
C	32.35149528499500	-27.59575267055284	7.06076772858666
C	33.61398009709345	-27.89551341670851	6.29466336393748
C	33.83686848035330	-29.35812796113877	6.11884022338548
O	34.75298613246722	-29.91531818760219	5.55314406357776
O	32.81795595729873	-30.12400904532517	6.68767841825026
H	29.66601752513047	-22.75401981921611	4.34222704249029
H	30.95904097252480	-21.97982487131351	5.26641840996953
H	29.88552033590576	-23.13830675779793	6.05339025263098
H	31.04844614657413	-24.41321909181688	1.49412140185563
H	30.01185932597147	-25.67079071190934	2.17107072457090
H	29.69146054351401	-23.97082388313811	2.53655144183055
H	33.63533785384933	-27.34819354482545	-0.11652763065044
H	34.42200969653955	-28.91230829682561	-0.35841009338658
H	32.86449499295607	-28.82215095145347	0.47344883465324
H	36.32345894467053	-29.76059811398204	0.26126389565968
H	37.68926463658404	-29.16345253889480	1.21237313775646
H	36.78664021722851	-30.57834133433748	1.75912334936937
H	33.57874582378966	-22.77239805920722	10.73341306940360
H	32.14868000639882	-23.15056263956532	9.76497905346073
H	33.33858652611388	-21.99431073713556	9.16369237707715
H	36.72469832445111	-24.47907880773174	10.80512823962599
H	35.61990755211642	-25.71447824561042	11.41077477099160
H	39.83007267715787	-29.04762444984663	8.67151900902169
H	39.38391817479958	-27.41754258650058	9.19246870360349

H	38.39499126556466	-28.79750721256273	9.67328675227284
H	39.07358591458765	-30.58985060058794	5.50029170801476
H	40.01938391748052	-29.16902346151492	5.04897726536675
H	40.17618670072069	-29.85486892167081	6.67130351515484
H	35.18382673864668	-24.00577625900477	11.53238031958942
H	33.42936058022099	-31.91734437090867	8.60864423266925
H	33.82103400486975	-33.25699310962337	7.51222226050197
H	34.83022109199935	-31.79813213128985	7.52616025997170
H	33.32705427301471	-31.76760481047724	5.54092558684136
H	31.90313469765169	-31.91327902680344	6.60029917517352
H	32.20245303689659	-26.53498516938553	7.22578980235594
H	31.47688656664890	-27.98702806512470	6.52275307620016
H	32.34820133717252	-28.10606305565949	8.03294140297342
H	32.32514859534327	-26.63735159479253	1.84623598118709
H	36.97081524804222	-26.68453360387254	9.50355441516566
H	37.81669093116343	-29.24959259026275	3.73694424139900
H	32.12450332446825	-23.22853268048545	7.22750613195024
S	36.05684820861271	-24.62815330787622	4.87114208868128
C	37.47438029722193	-25.16306942887541	3.83970514704993
H	38.16586983697070	-25.80080155419032	4.40310691230631
H	37.14224812004612	-25.72313567387041	2.95752591533208
H	38.02478578513256	-24.27832005236285	3.49757979132808

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B3LYP Scan/Thiolate IPC Model/RKS/190 degrees Constrained Optimization

C	30.47362204775093	-24.77788352649190	2.43802496454998
C	35.72442441010985	-24.66567494057077	10.88250883997229
C	39.52495836157326	-29.56447876832540	5.89387924925702
C	33.82392695385402	-28.39734928712129	0.41747799846294
N	33.11870382042358	-25.56014049367075	4.98636353739005
N	34.62255686177826	-25.52350219630131	7.39863427986062
N	34.95621823068365	-27.48062170510952	3.87825551234748
C	32.91332115896859	-26.65301587229146	2.80651013935787
C	32.74427903016200	-24.04784587463035	6.87151208461887
C	36.49405844299894	-26.57623107180244	8.57234132412191
C	37.09728496107114	-28.60602001148336	4.23166113762692
C	30.40663180535601	-22.97104690989884	5.14259095992028
C	33.25399232301195	-22.90153864040193	9.71008859370217
C	39.06065631591004	-28.28085285361469	8.85119128068545
C	36.68531267083326	-29.63845319768848	1.33805661515674
C	32.49836064846594	-25.75612958998432	3.78523784174789
C	33.75535234218177	-24.51515856192381	7.70793434442177
C	36.99100866137739	-27.35834137426937	7.53376145179545
C	35.98818766498955	-28.27409047831410	3.46302650637333
C	31.37120443630344	-24.84452732297073	3.63862094198840
C	34.00980294078965	-24.01871604913075	9.05322520132343
C	38.21566315804953	-28.14463573145892	7.61892142051110
C	35.75559381275033	-28.74515665206361	2.10530371166394
C	31.34368340312879	-24.08302004944058	4.77506770580745
C	35.04793650397124	-24.76102294220693	9.54708433843723
C	38.41230288195959	-28.68246637057546	6.37720338424918
C	34.55060559039910	-28.22478283911415	1.71857785131791
C	32.44294856700419	-24.54987389991046	5.60853634125096
C	35.42550588450887	-25.68948449283868	8.49038886867691
C	37.29298244266311	-28.23972587358732	5.55720612406812
C	34.07385553218953	-27.42234214845510	2.83750337687432
N	36.45258035777595	-27.44528364083870	6.28266162653291
Fe	34.73144819818669	-26.58644699791864	5.67095759078077
C	32.81050187674716	-31.51574242493275	6.23101174235339
C	33.48644819857936	-32.25267678409599	7.38126278910493
C	32.40626139420354	-27.61036673927941	7.13634094681675
C	33.65676614836585	-27.90038740277857	6.34721479930933
C	33.85809763429300	-29.35936648756196	6.12338468253445
O	34.83375171956754	-29.92362699090343	5.67867000972290
O	32.73169554111126	-30.10754798733598	6.46800540153112
H	29.64624129968855	-22.81199533296117	4.36974247332268
H	30.93942822199117	-22.01953646545387	5.27805733753322
H	29.87731620770922	-23.1755776601266	6.08394067873478

H	31.02548009142202	-24.49090552266040	1.53180652900392
H	29.99860454132456	-25.74636948317500	2.22716206372939
H	29.67185888384202	-24.04417621752248	2.57662805324594
H	33.61005266662124	-27.43161615761534	-0.06078676591073
H	34.40977225913331	-28.99049137145456	-0.29351869735136
H	32.85879978507865	-28.90662412510833	0.55115542490820
H	36.32010839131826	-29.82002561012008	0.32105119395090
H	37.69041134921413	-29.20282157391097	1.25254020344290
H	36.80256849047116	-30.61726185257991	1.82388155465002
H	33.61617651826366	-22.71487029993412	10.72715696364024
H	32.17893166402148	-23.11973567073351	9.78021367266273
H	33.35161629337973	-21.96164284424134	9.14919893519533
H	36.78120903606818	-24.38043014973825	10.78426681733924
H	35.70305953177063	-25.62414401457255	11.42015720655076
H	39.91553464715741	-28.94436512957570	8.68010526495610
H	39.45833350878792	-27.31188794158300	9.18448641736739
H	38.48819992670451	-28.69527124504425	9.69302416078122
H	39.14834732751091	-30.53302606958828	5.53685122959076
H	40.07148472812079	-29.10630052245900	5.05757619993099
H	40.25300941820139	-29.76898474929461	6.68695033578440
H	35.24270135276996	-23.92072085200195	11.52532388414441
H	32.97463855966373	-32.04877607501015	8.32628854275814
H	33.46881662665763	-33.33500308226181	7.20771374075949
H	34.52656207515768	-31.93628640413030	7.47271149753460
H	33.34641197458703	-31.69622214234997	5.29612851025012
H	31.77212528250880	-31.83977115827963	6.11695022850522
H	32.28816392840052	-26.55688770063766	7.36312470262502
H	31.52223618012204	-27.94528075864606	6.57741702627166
H	32.38796261948224	-28.17543720704566	8.07850292237900
H	32.31601343935206	-26.70367217757060	1.90081775918227
H	37.03776401133498	-26.60531296962893	9.51212831854745
H	37.84830982097386	-29.24321034598521	3.77443345880638
H	32.12559901939927	-23.23751083062196	7.24530695507762
S	36.05387128375902	-24.62313980534567	4.87510604094475
C	37.45664597451040	-25.15424614716389	3.82132730796264
H	38.16717014558649	-25.77625198328440	4.37862156424091
H	37.11402754532637	-25.72883833260999	2.95280080524880
H	37.98942912355877	-24.26707683079444	3.45815837147794

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B3LYP Scan/Thiolate IPC Model/RKS/200 degrees Constrained Optimization

C	30.44605176840897	-24.88671274429495	2.51499704764767
C	35.83370548950366	-24.52116904384604	10.86824836870781
C	39.60187867840794	-29.49766726481262	5.93415690894947
C	33.80434758316323	-28.51072254843965	0.51931090379701
N	33.12501558897926	-25.59884379546630	5.04876691483770
N	34.66354516812430	-25.49723147356878	7.43749944177259
N	34.97495864972324	-27.51791173981177	3.94625497748944
C	32.91185201354966	-26.72588650952579	2.88585143182426
C	32.747141116201576	-24.06781880979936	6.91713447945333
C	36.58407411702484	-26.47976163552317	8.59205286562230
C	37.12814276577503	-28.61930685556936	4.29633967974125
C	30.37750324136325	-23.04710943872007	5.19664798074504
C	33.29261089445631	-22.84772574042987	9.71748743564682
C	39.18073269099543	-28.13776778048591	8.86232384174974
C	36.68154227484413	-29.72169303297388	1.43071475240663
C	32.49645964214461	-25.81965723803726	3.85603118092332
C	33.78105696541277	-24.50043972798095	7.74377592962195
C	37.07214236163857	-27.27945878812255	7.56322362206073
C	36.00526364232249	-28.31464461007359	3.53523524464937
C	31.35489475123237	-24.92630557464578	3.70838833152985
C	34.05507400590236	-23.96638970524828	9.07079183984915
C	38.30872625321195	-28.04702549664340	7.64466658378907
C	35.75740004029581	-28.81670757759091	2.19112489054682
C	31.32593924988342	-24.15161576033778	4.83590061498500
C	35.12248739065421	-24.67171211545433	9.55611163084630
C	38.48673176687729	-28.61732093876686	6.41491160364583
C	34.54572391188221	-28.30861967520041	1.80792630393339

C	32.43940622165205	-24.59199921822288	5.66492059670950
C	35.49545632862500	-25.61763734391266	8.51315977171892
C	37.34526402982637	-28.21143065883659	5.60611713942105
C	34.07892101577404	-27.48519100345821	2.91555785875532
N	36.50948691147783	-27.40699546787481	6.32629214071172
Fe	34.76436314011304	-26.58884963393566	5.72807454029142
C	32.71025820635096	-31.42918056163387	5.80268953077014
C	33.84976851518396	-32.32520797348501	6.98737454182561
C	32.44592065521999	-27.63621096117066	7.19333483602212
C	33.70726643446917	-27.90911411940071	6.41394719958234
C	33.88271110983470	-29.35915268851495	6.12186854817567
O	34.89786772295377	-29.94930345363599	5.82563342231339
O	32.67145552112557	-30.04754164155507	6.17302283748607
H	29.60954817643282	-22.90728678672925	4.42753159274671
H	30.89945322958229	-22.08747553579282	5.31606398664994
H	29.85758056628078	-23.24607206065632	6.14441535759603
H	30.98907476895893	-24.61750705342811	1.59816078297400
H	29.97106933175650	-25.86025261027822	2.32841909138336
H	29.64411422892142	-24.15177158927745	2.64575554139095
H	33.57473318898671	-27.55531311999567	0.02794166321848
H	34.38718376396382	-29.10983506085193	-0.18916272844842
H	32.84614717546732	-29.02722196523017	0.67364497006548
H	36.30417551281034	-29.92582461674759	0.42243537691676
H	37.68343636061638	-29.28363926095386	1.32319339669944
H	36.80979119952097	-30.68981201709576	1.93485520165567
H	33.65746263790471	-22.64607073807785	10.73076924545510
H	32.21981585531874	-23.07388502864578	9.79463893415179
H	33.38021854208358	-21.91344668905560	9.14540755355676
H	36.86730965060254	-24.17216822180947	10.73407224927042
H	35.88851336912086	-25.47312395737838	11.41460056557949
H	40.03684244270712	-28.80029311146679	8.69382788739620
H	39.57797400175973	-27.15595436549469	9.15638323741088
H	38.62967672384785	-28.52937933574713	9.72888027623404
H	39.23041521347073	-30.47587260301471	5.59894372648468
H	40.13507335135624	-29.04965897722936	5.08375047080237
H	40.34064399635589	-29.68139146885065	6.72244349228802
H	35.32733351919693	-23.80039239016608	11.51971435883052
H	32.35193611448867	-32.15657499966964	7.81288041360020
H	32.99213423105223	-33.38151309639706	6.69975932739716
H	34.06201109509531	-32.11980490662681	7.33957044741099
H	33.43595562254027	-31.56677746589412	4.99797616210142
H	31.70828441771021	-31.64755432620073	5.42280120592748
H	32.39519522240787	-26.61569055213113	7.55885129288876
H	31.57541881562071	-27.81002206439076	6.54645141880984
H	32.32720018030913	-28.32406153808906	8.04116340621232
H	32.30426601380047	-26.79730779861861	1.98844382599904
H	37.14904372005830	-26.47420638334366	9.51964418936316
H	37.87698641000841	-29.26278636852039	3.84442798880991
H	32.11954016094978	-23.26244808898696	7.28682304444420
S	36.02969147325800	-24.62195693714617	4.85393887706245
C	37.43446133863955	-25.15690187696719	3.80421385004790
H	38.16665224446869	-25.73991046093025	4.37528678432922
H	37.09732557483027	-25.77066285463196	2.96062842419672
H	37.94064936233895	-24.27041147047533	3.40329974653548

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B3LYP Scan/Thiolate IPC Model/RKS/210 degrees Constrained Optimization

C	30.42093324198982	-24.97025051695154	2.57543655506309
C	35.91660795695911	-24.40245512772712	10.84870272552433
C	39.63768103055870	-29.47486689340485	5.97646653342031
C	33.78475679693904	-28.59716714632539	0.59822135583195
N	33.12467387958266	-25.63049215349635	5.09721744889916
N	34.69042736511956	-25.47578767431965	7.46636179717229
N	34.97638602652505	-27.55846485363834	4.00435595135367
C	32.90440594039239	-26.78407735961211	2.94812734462774
C	32.74624443819612	-24.08239458656787	6.95141801154455
C	36.64725288999936	-26.40475590396008	8.60436934581473
C	37.13247359250582	-28.65265976964361	4.35690166457517

C	30.35128677566013	-23.10634206853420	5.23927267496896
C	33.32323324711345	-22.79870196022555	9.71713601496393
C	39.26075569664369	-28.03634706257726	8.87170262239492
C	36.66568512739384	-29.79957025263918	1.50991884174416
C	32.48979632575161	-25.86997342668510	3.91128342004409
C	33.79830368734760	-24.48640988607148	7.76940732653126
C	37.12432932160743	-27.22530913844598	7.58724322219338
C	36.00304423634061	-28.36269701659454	3.59908562765959
C	31.33806222078719	-24.98981745616092	3.76304778868594
C	34.08916764148601	-23.92033804517419	9.07965666078437
C	38.36631331154069	-27.98408798143393	7.66801993621099
C	35.74568168753171	-28.88535413023251	2.26455977320506
C	31.30807572095348	-24.20533141027885	4.88367797629655
C	35.17848592825226	-24.59680405579448	9.55717547379513
C	38.52527983681499	-28.58820659234326	6.45202801275400
C	34.53249354101042	-28.38022232094964	1.88085292907468
C	32.43235350240011	-24.62562313232837	5.70880821880938
C	35.54553782414698	-25.55924040446719	8.52705966757538
C	37.36800758199193	-28.20940024258945	5.65213507616552
C	34.07334260619839	-27.54032373990484	2.97900314876809
N	36.54139436348696	-27.38834857361123	6.36385149984324
Fe	34.78087812157352	-26.59548209632094	5.77439672873171
C	32.67611494616861	-31.30724363531047	5.46434441471331
C	32.78609933189644	-32.32617037352853	6.59118247243318
C	32.49135197809817	-27.65431967830681	7.28503646260414
C	33.74113384847109	-27.91251491539194	6.48271443470405
C	33.89367773847833	-29.35490804586944	6.14316285575587
O	34.91317294244398	-29.98500580294584	5.97689534530313
O	32.65659118261271	-29.96303448427694	5.95835095453856
H	29.57356926163430	-22.98604624233661	4.47666777992196
H	30.86378087999745	-22.13937097870698	5.33916835102463
H	29.84392053526626	-23.29729339920918	6.19543143991215
H	30.95558774462081	-24.70603365449213	1.65228210184727
H	29.95281249307146	-25.94952279566007	2.40202924654656
H	29.61394208481677	-24.24050577548083	2.70412472811835
H	33.56408791439755	-27.64809606316688	0.09067415965827
H	34.35875103618890	-29.21504549702425	-0.10128323788378
H	32.82140016311003	-29.10005236574627	0.76448056767729
H	36.27878446326434	-30.02192553477431	0.50913044224341
H	37.66451003542144	-29.35925707893897	1.38450683831515
H	36.80371171998741	-30.75866175017442	2.02845899612962
H	33.69408256541627	-22.58118272447031	10.72498332502248
H	32.25276858288924	-23.03146650208287	9.80517929707590
H	33.39997507279076	-21.87121446715570	9.13242385136635
H	36.93223176884896	-24.01574526014648	10.68379525302210
H	36.02205028934605	-25.34428115323017	11.40487002664060
H	40.11716952684585	-28.69910138679904	8.70588759689098
H	39.65805519025213	-27.04480379166035	9.13097048261024
H	38.72799948125369	-28.40633607145440	9.75891384606199
H	39.26609950520393	-30.46144343760258	5.66703286574449
H	40.15903929661010	-29.04335714215792	5.11028388087244
H	40.38668708124864	-29.63878146238968	6.75947355319926
H	35.39948646672546	-23.69306066688366	11.50430270674432
H	31.98620725789925	-32.18241489891397	7.32366322648707
H	32.71020634312498	-33.34589122355478	6.19600926290760
H	33.74651148448621	-32.22469192027621	7.09934739952762
H	33.50571952638732	-31.42017243936929	4.76287929037028
H	31.73293852028176	-31.42080359284259	4.92311991802159
H	32.45954204753905	-26.64864484345182	7.69297343539040
H	31.61655837562920	-27.78763066943563	6.63514966710625
H	32.36784703908182	-28.37494615603910	8.10565627599627
H	32.29056474038178	-26.86894310062114	2.05617603123322
H	37.22947552001817	-26.36994549672712	9.52057470562514
H	37.87676111511519	-29.30607898503163	3.91175028524127
H	32.11246316372107	-23.27997702616431	7.31705796387029
S	36.01368837093309	-24.63657914796838	4.84046358334815
C	37.41444678792983	-25.18516211853282	3.79179394571752
H	38.15715368534050	-25.74698793372474	4.37044051668467

H	37.07636817664767	-25.82151675392231	2.96555829604145
H	37.90903794190853	-24.30380867704013	3.36572418858953

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B3LYP Scan/Thiolate IPC Model/RKS/220 degrees Constrained Optimization

C	30.39731068617969	-25.01229998134762	2.62229310740179
C	35.96764490860269	-24.32668801130266	10.83719619059466
C	39.63349939507420	-29.48911982168751	6.01141615910085
C	33.73531001993461	-28.67612649261484	0.67014242924506
N	33.12162292967592	-25.63908210959403	5.13080864879299
N	34.70929601210845	-25.45000900898935	7.48280176448559
N	34.96346904908602	-27.58634484850699	4.04711089100948
C	32.88593331635870	-26.81859064367523	2.99673885634660
C	32.74868994102300	-24.07749994220038	6.97462261963547
C	36.68738026810285	-26.34963785268170	8.60789648138248
C	37.11491645998520	-28.68814869795313	4.40284269563407
C	30.33889584248357	-23.12479108064505	5.26911213540014
C	33.34381996309368	-22.76181390945089	9.72177471998100
C	39.29946998136888	-27.98424995456968	8.87761741934373
C	36.61449773894772	-29.88529126257014	1.57921633214628
C	32.47896653158335	-25.89254352933186	3.95188466961441
C	33.81119416752016	-24.46626889123651	7.78632517509239
C	37.15420923236513	-27.18631124011087	7.5992670069715
C	35.98075463137010	-28.40586006323087	3.64826098821041
C	31.32308780632301	-25.01775465682100	3.80336992496480
C	34.11258312145005	-23.88303161637085	9.08693540613403
C	38.39294173452351	-27.95025849474874	7.68233882395156
C	35.70723419249265	-28.95197641923223	2.32628032182862
C	31.29724253296443	-24.22368047899970	4.91730559258861
C	35.21513864821814	-24.54257188772808	9.55734914457746
C	38.53372614774005	-28.58263224584258	6.47871673214488
C	34.49487826567173	-28.44307306065078	1.94313274307875
C	32.42908026690611	-24.63215407472707	5.73823769868670
C	35.57863245351455	-25.51303191658664	8.53320147690719
C	37.36964449059565	-28.21371848021402	5.68374020028766
C	34.05151916209045	-27.57975371657407	3.02909789214775
N	36.55742510228336	-27.37043972335713	6.38575318979445
Fe	34.78932059945411	-26.58878622754463	5.80505743681454
C	32.80100547101502	-31.20630461973510	5.20183099042056
C	32.65469858472840	-32.28193302535084	6.26972480672454
C	32.50141395184150	-27.66307006639215	7.31951992059435
C	33.76374213538767	-27.90013052821233	6.53160497902706
C	33.93353070363937	-29.33851819411334	6.18640238074078
O	34.94871298970777	-29.99586441409955	6.18971037270888
C	32.73340101144404	-29.88726635520532	5.75995184912511
H	29.55251462537320	-23.01806643749822	4.51339227151281
H	30.84763756088377	-22.15412503066035	5.35105633846407
H	29.84267925130402	-23.30579817712354	6.23301785962029
H	30.92462721108695	-24.75646203461545	1.69261943994425
H	29.92990649896291	-25.9942077237773	2.46232715232022
H	29.58981786473039	-24.28283151912789	2.74943882828382
H	33.52950942670793	-27.73529923639805	0.14135149551624
H	34.29313845119209	-29.32123052041121	-0.01772160851252
H	32.76354432337658	-29.15605719269131	0.85390694645820
H	36.21237398949262	-30.12937407088590	0.58954500734464
H	37.61213982882745	-29.45013033936680	1.42878773476401
H	36.75915031513083	-30.83280994370281	2.11686953406793
H	33.72152116543934	-22.53361600227836	10.72472577059223
H	32.27582139802481	-23.00140205626829	9.82060601728058
H	33.40908955368356	-21.83840490850230	9.12920025409465
H	36.97502159606901	-23.92610499036347	10.65569482483518
H	36.09468888929542	-25.26237108926874	11.39913671451328
H	40.15194627886120	-28.65276880827279	8.71478192651620
H	39.70257598266924	-26.98975594565152	9.11563818673572
H	38.77458320263843	-28.33710840393277	9.77643372410614
H	39.25038442774579	-30.47972687117686	5.73017991638792
H	40.14804065233707	-29.08264647681692	5.12921831405322
H	40.39032549729600	-29.64047028909688	6.78941998702945

H	35.44861213405505	-23.61990304461420	11.49414550798059
H	31.72709673870547	-32.14613884591297	6.83373870068121
H	32.63517208377417	-33.27763808522178	5.81156252294759
H	33.49453119754325	-32.24147155174962	6.96565645684663
H	33.74551994860465	-31.31941886934745	4.66627025024700
H	31.97754327930593	-31.24888931156170	4.48418827220825
H	32.44556854112480	-26.65675627762160	7.72495519817959
H	31.63945090029572	-27.81577448910031	6.65717405780937
H	32.38348829987929	-28.38377307594252	8.14201557179306
H	32.26439472119588	-26.91409733387059	2.11120542604052
H	37.28020281400318	-26.29856540301411	9.51651370197516
H	37.84970623535940	-29.35756234990242	3.96569731681972
H	32.11261992062035	-23.27609975500189	7.33860962749637
S	35.99900652092192	-24.64543484761163	4.81267170011334
C	37.41465233182269	-25.21705736082979	3.79630440112158
H	38.15518707040283	-25.75575501561234	4.39914739240057
H	37.08972401229502	-25.87989051420756	2.98577357550620
H	37.90813149710560	-24.34565830818394	3.34886792254184

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B3LYP Scan/Thiolate IPC Model/RKS/230 degrees Constrained Optimization

C	30.39168303216056	-24.99566473800311	2.63301540382934
C	35.99379135704697	-24.28900160110531	10.82475742612056
C	39.59469414301005	-29.53296870797667	6.03222508500760
C	33.69226586329248	-28.69973585680776	0.69782390350361
N	33.10994961869763	-25.63579642228638	5.14495679972796
N	34.71110527577270	-25.43596546532785	7.48731429222931
N	34.93810181715358	-27.60078251263107	4.06531875957398
C	32.86656272177175	-26.81872659071174	3.01352482333047
C	32.74608890183351	-24.06769217504923	6.98501501099771
C	36.69827321469771	-26.32670750335999	8.60323356178650
C	37.07832459336998	-28.72311028965175	4.42574280180924
C	30.34089762349457	-23.10584737294741	5.27829554584066
C	33.35764061853768	-22.73718586187902	9.72116028933537
C	39.29715983778576	-27.98120321366610	8.87739104001082
C	36.55808060573368	-29.93698148421097	1.61085401796868
C	32.46648368935369	-25.88719504450970	3.96599911768061
C	33.81340004873439	-24.45249859060235	7.79222338848118
C	37.15437071484261	-27.17549242993074	7.59982704444396
C	35.94526281804794	-28.43547355211895	3.67075678775580
C	31.31572615127841	-25.00587245322291	3.81536457643968
C	34.12363175829572	-23.86068329498045	9.08696703807217
C	38.38523149623897	-27.95174423079668	7.68613205652662
C	35.66262757953819	-28.98878446380737	2.35374997923796
C	31.29250877535914	-24.21137890995342	4.92891231590256
C	35.23166898356867	-24.51448758500134	9.55225542405912
C	38.51055538686720	-28.60403735103058	6.49164127611106
C	34.45604846140690	-28.46709045463570	1.96845829990526
C	32.42196550281914	-24.62492530373192	5.75075358099968
C	35.58901772158815	-25.49052781022129	8.53105993093795
C	37.34608398964065	-28.23258537712879	5.69823603112480
C	34.02470862261887	-27.59093810837966	3.04856255961722
N	36.54868612747470	-27.36875503302669	6.39224010492561
Fe	34.78037355543569	-26.58420009578008	5.81669341381116
C	32.94933361465326	-31.16623947202976	5.07564474950071
C	32.68617376441986	-32.25092879767821	6.11178517584169
C	32.51322844870143	-27.67599011253824	7.36592230249709
C	33.76664702356322	-27.88996997477677	6.55913749666978
C	33.95873105548525	-29.32832653695050	6.22791620905939
O	34.95295969276315	-29.99997800233715	6.37967764990270
O	32.82517187450365	-29.84994516288133	5.63497711607819
H	29.55425857580274	-22.99703995913417	4.52313609023333
H	30.85543322746195	-22.13789269140682	5.35633805534821
H	29.84470254086694	-23.28057114874231	6.24336887382617
H	30.92320191298933	-24.74987032818974	1.70307471266934
H	29.91363397190602	-25.97309066858074	2.47674838678593
H	29.59212334899494	-24.25671301061583	2.75554666939865
H	33.50149439442132	-27.76052659326437	0.16052326967800

H	34.23943216665119	-29.35990059183456	0.01573874346842
H	32.71284518936270	-29.16195084076710	0.88610061034795
H	36.14831490475664	-30.18722413175633	0.62586776443536
H	37.55832164182736	-29.51140829975187	1.45044088681482
H	36.69875788549749	-30.88071569623093	2.15625583013261
H	33.74002531327478	-22.50531291086043	10.72150707617195
H	32.29006853974600	-22.97619118391051	9.82568117193909
H	33.42033887422991	-21.81587306271378	9.12497986536800
H	36.99409374823163	-23.87516149629167	10.63390386115566
H	36.13830213083111	-25.22308671299279	11.38496158627078
H	40.14494007756395	-28.65603166139567	8.71613956861865
H	39.70702486062636	-26.98718656460903	9.10546458107096
H	38.77437034524983	-28.32385216914636	9.78139756808230
H	39.19624479149857	-30.52325544391498	5.77187379263423
H	40.10763963792981	-29.14925338089865	5.13899493883833
H	40.35543177320516	-29.68049541747996	6.80712949294184
H	35.47188164881238	-23.58923390034995	11.48699342224212
H	31.70305157767813	-32.11771589005863	6.57303061570169
H	32.71511075370736	-33.24207896325596	5.64444394486494
H	33.44646156187338	-32.21690597542742	6.89360114659026
H	33.94600653975512	-31.27671905037345	4.64427854074758
H	32.20889212352110	-31.19695504485340	4.27264748547365
H	32.40445477955812	-26.65160742636914	7.71106906057317
H	31.64403379558416	-27.93043922416157	6.74533310360372
H	32.47184617724582	-28.34675492916466	8.23795053506521
H	32.24404508804760	-26.91168302878115	2.12837574962793
H	37.29804382650678	-26.26912410501539	9.50688113796674
H	37.80309335730249	-29.40724745478781	3.99465999112796
H	32.11243324427038	-23.26428219851308	7.34881116639229
S	35.98852565182182	-24.65303283062553	4.80008933625477
C	37.40567802068372	-25.24563481389677	3.79734250339797
H	38.14123156327295	-25.77961286731709	4.41033868096838
H	37.08093984917340	-25.91730537758673	2.99404799501116
H	37.90554119170141	-24.38292511130850	3.34012420750607

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B3LYP Scan/Thiolate IPC Model/RKS/240 degrees Constrained Optimization

C	30.38148378892435	-24.99378017970893	2.65007985624404
C	36.02465536574407	-24.26480352708488	10.81209137575081
C	39.57701154959678	-29.56195193601222	6.03760363317943
C	33.67383186780837	-28.69967049262918	0.70608780513739
N	33.10886201135312	-25.63167222604973	5.15282056058116
N	34.72127258025991	-25.42586842224257	7.48733771961578
N	34.92788976020150	-27.60600340954210	4.07227324258035
C	32.86162569658644	-26.81118358092888	3.02018906430809
C	32.74650368062441	-24.06776975055714	6.99693292418038
C	36.72105024428478	-26.30494903247803	8.59047307540052
C	37.05338227444238	-28.75494735221201	4.43993149966761
C	30.32881520999912	-23.11448803193515	5.30308113242626
C	33.36949891768808	-22.73199558052006	9.72814241749633
C	39.31840072224909	-27.96247507901853	8.85994203108183
C	36.52011192062982	-29.97321083069666	1.62867774268261
C	32.46326604198235	-25.88137823912026	3.97468821615934
C	33.82082767883033	-24.44695199500753	7.79756860335409
C	37.16740509296272	-27.16412169217258	7.59151410978139
C	35.92347404138567	-28.45744316206649	3.68324243055622
C	31.30904923794365	-25.00351306700571	3.82965217862528
C	34.13790008816993	-23.85098026240981	9.08892555467884
C	38.39462116327019	-27.94609649017493	7.67758294865526
C	35.63511949426634	-29.01252920585236	2.36812661972891
C	31.28519274955298	-24.21343287493542	4.94615798512875
C	35.25406043106545	-24.49659306962258	9.54580399566279
C	38.50347087407955	-28.61884776381190	6.49291572988316
C	34.43675538169105	-28.47507334080067	1.97881709085046
C	32.41918828507318	-24.62486737207744	5.76321641000882
C	35.60831325554179	-25.47314594816779	8.52380370093732
C	37.33427144709329	-28.25107505840610	5.70467334468924
C	34.01509535018413	-27.59022167750995	3.05569214603132

N	36.54991078369746	-27.36998393510693	6.39202692015885
Fe	34.78197513956124	-26.57936403517670	5.81951214937026
C	33.09254024027805	-31.15339656168896	5.01737222852750
C	32.56053493509415	-32.20152067732442	5.98495728471361
C	32.53073264118859	-27.68131190582229	7.39546257276689
C	33.77560791016571	-27.88125161405600	6.57382165276599
C	33.98634788373802	-29.32429248638143	6.27673181713714
O	34.93518803797376	-30.00978026321024	6.58099253409074
O	32.93540782738238	-29.82514095610486	5.54026997524619
H	29.53796333250198	-23.00827108142335	4.55196405178662
H	30.83778937034541	-22.14361528006482	5.38157902689097
H	29.83831042710585	-23.29508145365264	6.26998475915648
H	30.90855752074594	-24.73959785524951	1.71985027964193
H	29.91001072687265	-25.97380350526703	2.49028800944123
H	29.57707158808585	-24.26114327461662	2.77862515913027
H	33.50353304444504	-27.75981716176407	0.16297633901484
H	34.21114012991146	-29.37376470566277	0.02982206249937
H	32.68476177781421	-29.14171443568228	0.89212204185460
H	36.10753626376775	-30.22267971283479	0.64466808531822
H	37.52480918737983	-29.55891349755797	1.46645042163371
H	36.65123552711830	-30.91669750309327	2.17698695763614
H	33.75706314983402	-22.49793770834394	10.72599948764174
H	32.30411386868557	-22.97752729329283	9.83970209235585
H	33.42261499025018	-21.81018674900071	9.13179867078466
H	37.02060962925326	-23.84431439091575	10.61321907073302
H	36.17978593999010	-25.19752093415478	11.37169457410212
H	40.16408948227716	-28.63979715451598	8.69815110456037
H	39.73114098799192	-26.96617989376298	9.07213068100169
H	38.80454050385367	-28.29418459471809	9.77309440136599
H	39.17069735741243	-30.55535668096628	5.80227697211138
H	40.07978083376892	-29.19844278175012	5.13027448804778
H	40.34730678617071	-29.69775313402806	6.80515653700541
H	35.50307022973748	-23.56813308560456	11.47785110088337
H	31.51981994319786	-31.99326016991614	6.24954147284248
H	32.60595442431339	-33.19933099058113	5.53347997957213
H	33.15708438185200	-32.21114565020094	6.89927322242596
H	34.14732161755164	-31.32736822552259	4.79810505743388
H	32.52873323713503	-31.15337073593447	4.08174663412608
H	32.36103394390040	-26.64244972799682	7.66392114585030
H	31.66272865632317	-28.04685346673669	6.83015615662227
H	32.56811497710456	-28.27936597908382	8.31978499220240
H	32.23821492935550	-26.90170651757704	2.13539815901827
H	37.32898038873589	-26.23953253244003	9.48811541965646
H	37.76856982910054	-29.45188134589591	4.01323942952521
H	32.11105655929675	-23.26748305503261	7.36450403389990
S	35.98874883216222	-24.65817716291944	4.78696144627287
C	37.40766505045718	-25.26601698651189	3.79552311944847
H	38.14019680142282	-25.79502972052244	4.41640119605504
H	37.08386670372190	-25.94520937548641	2.99816525549966
H	37.91121215148435	-24.40958150408916	3.33053903110987

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B3LYP Scan/Thiolate IPC Model/RKS/250 degrees Constrained Optimization

C	30.37631009656441	-24.96033643313328	2.65564568827363
C	36.04357079206677	-24.26906316362265	10.80431581744985
C	39.54475614756286	-29.60160610993121	6.02682671843540
C	33.64047811763468	-28.68792475895209	0.70329365796569
N	33.10889912668142	-25.61233425774137	5.14897258190124
N	34.72924247045336	-25.41600250474660	7.47886952580938
N	34.91832543952142	-27.59039751376986	4.05906229674575
C	32.85644806643358	-26.78043742527408	3.01098078249617
C	32.74782136548814	-24.06204037269601	7.00485831916625
C	36.73533694874510	-26.29650458234139	8.56991130132629
C	37.02287083242906	-28.77604782167768	4.43399187966288
C	30.32318814190729	-23.10290849670955	5.32473239525051
C	33.37576691705631	-22.74268345697278	9.74322704268268
C	39.32171230467156	-27.97152206861998	8.83489371350540
C	36.46617044118973	-30.00276334183900	1.63087790103793

C	32.46171152117051	-25.85397809844461	3.97014571330669
C	33.82637638855214	-24.44278439117585	7.79914002290632
C	37.17248325891721	-27.16084164838573	7.57150225552516
C	35.89746490493918	-28.46298246708641	3.67600791375978
C	31.30609287000597	-24.97652740521776	3.83336006474048
C	34.14695600262935	-23.85316685219227	9.09267961702867
C	38.39219002590232	-27.95448254764774	7.65708885629461
C	35.59792369970229	-29.02304995573772	2.36519976055626
C	31.28228531070580	-24.19559038074956	4.95621319768456
C	35.26866853588405	-24.49586462392388	9.53976987839681
C	38.48623855163468	-28.64002743198500	6.47851321533959
C	34.40901182477975	-28.46725399521653	1.97334980658922
C	32.41887785151798	-24.61091872794494	5.76786711840964
C	35.62163001444587	-25.46550491257050	8.51068366170399
C	37.31723055299869	-28.26536420933013	5.69327919636648
C	34.00335375513765	-27.56875324989064	3.04530151693635
N	36.54685629299701	-27.36882228463716	6.37654714670624
Fe	34.78233818325442	-26.56477245953094	5.80657852068636
C	33.27473355222347	-31.19792292542586	5.05093334808037
C	32.50509171620427	-32.15315994393617	5.95269001324480
C	32.53377749910931	-27.68287642788854	7.38256076349918
C	33.78211651286195	-27.86795582513532	6.56348012921980
C	34.02764594564889	-29.31521411576509	6.32407427152046
O	34.91437649484279	-29.98832415050141	6.79779729842358
O	33.09158173716771	-29.83367484021560	5.46234641689023
H	29.53030031188345	-22.99272689018331	4.57635483595376
H	30.82902925609490	-22.13104357654853	5.41077378957035
H	29.83554403909316	-23.29379977011466	6.29111926880187
H	30.90058417399736	-24.69554894246425	1.72679624176340
H	29.90910274380990	-25.94107864884784	2.48793754596928
H	29.56871544365364	-24.23264012104923	2.79208476124510
H	33.48350376654606	-27.74901572600013	0.15455701861505
H	34.16621442472951	-29.37435730301430	0.03035232816734
H	32.64513832636948	-29.11347964224492	0.89410416029135
H	36.04736405820188	-30.25315657874953	0.64973046759365
H	37.47681694612822	-29.60540809281686	1.46311246551061
H	36.58417881103482	-30.94417115782074	2.18571538414434
H	33.76741874047605	-22.51282762274001	10.74047747971091
H	32.31242312990588	-22.99510621853105	9.85903484224155
H	33.42024239133639	-21.81667551711853	9.15273344906552
H	37.03739095821737	-23.84415715460436	10.60422975124334
H	36.20383943080912	-25.20473764608462	11.35747854158682
H	40.16381107820051	-28.65284435038323	8.67108830248882
H	39.73955347612742	-26.97636697632351	9.04215974903764
H	38.81081521495869	-28.29861276679288	9.75137014832049
H	39.12551744267898	-30.59475256932323	5.81361993968635
H	40.04037264924086	-29.25923498580816	5.10749499670943
H	40.32259948368846	-29.73230297769909	6.78759186114161
H	35.52225055420911	-23.57825008579142	11.47635648201263
H	31.44600541248698	-31.88223314568975	5.99192373811889
H	32.58205304142881	-33.18099459381012	5.57987424167361
H	32.90741344589505	-32.12638089844484	6.96767610138133
H	34.34048457105203	-31.43095703242768	5.05660284304067
H	32.90643908790533	-31.23340403299027	4.02343233815586
H	32.34150326803670	-26.64415119833200	7.63679347655127
H	31.67298502060270	-28.07243391822553	6.82044615054838
H	32.58481845467633	-28.26920678756689	8.31347236724893
H	32.23088659895647	-26.86644797691118	2.12724273777393
H	37.34786805897053	-26.23206907098370	9.46449814072296
H	37.72564306494772	-29.48736604205719	4.01025573400616
H	32.11123266364547	-23.26615493471917	7.37996244443756
S	35.99242824537422	-24.65096475522327	4.77046839983200
C	37.41767336138105	-25.27240822909248	3.79640538301128
H	38.14404052737839	-25.79749027464387	4.42778256605854
H	37.09806258600022	-25.95803281045628	3.00286225729385
H	37.92731221323059	-24.42190289880827	3.32717234974873

B3LYP Scan/Thiolate IPC Model/RKS/260 degrees Constrained Optimization

C	30.37873772304940	-24.93015581870367	2.65189869839044
C	36.05911779991194	-24.25981220800600	10.79286636898068
C	39.50888197711635	-29.64240730039787	6.03445419663053
C	33.62964281754903	-28.66573591456773	0.69331094139518
N	33.10280897319805	-25.60406880439275	5.14864382530628
N	34.72497842048853	-25.41661288704421	7.47847022872687
N	34.90395961234133	-27.58783623798967	4.05677656098479
C	32.85197927322694	-26.75992039942172	3.00404745908860
C	32.74668980058521	-24.05677821528408	7.00801131792846
C	36.73295814547451	-26.29930883410472	8.56473410125037
C	36.99038677104702	-28.80279263090333	4.44134039939301
C	30.32458991864017	-23.08667254850578	5.33103140919586
C	33.38870107901112	-22.73201338674304	9.74008934692216
C	39.31046533418580	-27.98766368226672	8.83005767104416
C	36.43637734982990	-30.01322351721077	1.63163371617409
C	32.45783297804326	-25.83715116872258	3.96697006156313
C	33.82632137584547	-24.43978670992435	7.79974092198957
C	37.16067727337021	-27.17281179390564	7.57045256952161
C	35.87324605381691	-28.47252988944614	3.67795399192960
C	31.30542645649460	-24.95518203701090	3.83186098175526
C	34.15425410539446	-23.84657733271353	9.08981566372333
C	38.37500923542898	-27.97439602734253	7.65690057717331
C	35.57427317294920	-29.02686880122718	2.36432145001943
C	31.28140169234027	-24.18003504603409	4.95865574253553
C	35.27692187574302	-24.48992312114088	9.53340382177930
C	38.45872387302242	-28.67054097273984	6.48363385587749
C	34.39427019012655	-28.45635001768744	1.96753085906721
C	32.41531256147697	-24.60258982938852	5.77036782916483
C	35.62206707362185	-25.46453798360581	8.50632361490294
C	37.29006261845256	-28.29217668894130	5.69976695782396
C	33.99356457096549	-27.55549041621189	3.03966712198942
N	36.52872029679568	-27.38491468725626	6.37921083890485
Fe	34.77049631566777	-26.56642669441259	5.80517691171619
C	33.39415301111513	-31.21470266078479	5.04468516413668
C	32.54734290275667	-32.13932520915959	5.90823902112890
C	32.52837199125106	-27.67589932124453	7.39927652700768
C	33.76420848884601	-27.86622004191247	6.56240419210200
C	34.01089480657325	-29.31918168375112	6.36300139037470
O	34.80561510996078	-29.99830683735068	6.97423609159319
O	33.19048926022837	-29.83574357538772	5.39609005082941
H	29.53415581789183	-22.96964453677971	4.58111130191200
H	30.83305945190481	-22.11685007622209	5.42427009925444
H	29.83369761956250	-23.28182538867978	6.29493052649786
H	30.90537847143429	-24.65784273428041	1.72654089391796
H	29.91258071713429	-25.90981432384099	2.47527212922033
H	29.57034255219637	-24.20400457163406	2.79182142099925
H	33.48463482815431	-27.72379901435675	0.14646475756114
H	34.15162577145398	-29.3555909292238	0.02090774937087
H	32.62927163495953	-29.08182184121269	0.87856337449992
H	36.01919365868297	-30.25798007409872	0.64837688704096
H	37.45119451496385	-29.62453397507619	1.46848451388949
H	36.54403148278179	-30.95681647696868	2.18487451940334
H	33.78735080724579	-22.49775932323773	10.73353767115319
H	32.32586273844919	-22.98260243753006	9.86430634628823
H	33.43031054526482	-21.80902169784027	9.14470905267800
H	37.05425581426454	-23.84169359675966	10.58518330396351
H	36.21697568032455	-25.19286439740818	11.35115262851388
H	40.14701261719560	-28.67622721328292	8.66804472292792
H	39.73626640328353	-26.99361730609568	9.02610221599179
H	38.80208387190427	-28.30300719766587	9.75197862054262
H	39.08251466859892	-30.63451690755969	5.83045407709434
H	40.00254400557741	-29.31014144204178	5.11038264081888
H	40.28930187091360	-29.77239582629688	6.79266663966298
H	35.54491035640366	-23.56187150997712	11.46300742542879
H	31.49125590056112	-31.85861997660607	5.85777941794900
H	32.64212735429085	-33.17718067281871	5.56867378759020
H	32.87078053712978	-32.08884742236872	6.94990560863020

H	34.45479646543622	-31.45264422883467	5.14168837310709
H	33.11014713192540	-31.27676471009169	3.99217538703150
H	32.33555261602785	-26.63507911278231	7.64443711459468
H	31.65776441595289	-28.07482241924100	6.85752550515526
H	32.60134456538479	-28.25219540203231	8.33455320671490
H	32.22917452459610	-26.83843522616381	2.11765723111477
H	37.35005322984080	-26.23214611022261	9.45596501266963
H	37.68580909645574	-29.52238252988989	4.01934011970622
H	32.11309895140530	-23.25914364066070	7.38448311243780
S	35.99199948102167	-24.66008443139419	4.77024206996112
C	37.41710417590018	-25.29321089497387	3.80339538169363
H	38.13913794142848	-25.81919798276235	4.43902018894753
H	37.09655327671614	-25.98043801781246	3.01161337121512
H	37.93229883443804	-24.44720542673176	3.33206354882790

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B3LYP Scan/Thiolate IPC Model/RKS/270 degrees Constrained Optimization

C	30.38665980495863	-24.87378379619610	2.62790203727808
C	36.05118633837784	-24.26457849707980	10.78411577889655
C	39.43883614417896	-29.70968455697432	6.04870772474615
C	33.60586802824839	-28.63947953247467	0.67542620600327
N	33.09004702893522	-25.58595870229782	5.13650732208036
N	34.71124539761215	-25.41158402938577	7.46866257883950
N	34.88258688718416	-27.57402753139474	4.04192746765127
C	32.83970847002479	-26.72928327491691	2.98557538858931
C	32.74277612673479	-24.03825498923281	6.99749781435038
C	36.70911499794664	-26.31294274068347	8.55866811633638
C	36.94993045271687	-28.81856740120506	4.43560514650974
C	30.33594014705151	-23.04139719308581	5.31475843895719
C	33.39292401420425	-22.71710292017606	9.72872231761224
C	39.25452190099918	-28.04720587787007	8.84114770090850
C	36.39825465726447	-30.01318678358318	1.62020822488522
C	32.44873266971509	-25.80762654744355	3.95090309170278
C	33.81945369169993	-24.42850738962355	7.78950860899460
C	37.12932017995259	-27.19269986934896	7.56677326719920
C	35.84291211484177	-28.46864809528168	3.66593197713022
C	31.30537543888180	-24.91428207991613	3.81363282428253
C	34.15101102879151	-23.83736369850349	9.07945463477276
C	38.32866230302169	-28.01552587274499	7.66089285466900
C	35.54327254182387	-29.01878084331550	2.35042483866969
C	31.28302131567967	-24.14356557368119	4.94343544633426
C	35.26855892262800	-24.48900918644815	9.52393375688640
C	38.40695975717085	-28.71444659179635	6.48875816262576
C	34.37011185132312	-28.43695499147105	1.95081313802827
C	32.40919942456622	-24.57995190858421	5.75861810556683
C	35.60693155958054	-25.46666022404144	8.49740142416368
C	37.25086280959307	-28.31499984447006	5.69704113405351
C	33.97508073170157	-27.53310580947193	3.02283813955180
N	36.50104665287321	-27.39477052214233	6.37159055644911
Fe	34.75100033849322	-26.55962452213086	5.79268744455490
C	33.59643129654932	-31.24940488436333	5.09385881587423
C	32.66119267667459	-32.15352169216256	5.88474686471612
C	32.53903131481638	-27.66880819040086	7.43254061579044
C	33.75119882215051	-27.85820429810201	6.56171341337663
C	34.03023583973181	-29.31237924124419	6.42000660617672
O	34.74134341697633	-29.96639424810546	7.15205652710750
O	33.34640125125694	-29.86103107384196	5.37275768303319
H	29.55089215810569	-22.91315316608099	4.56103283197202
H	30.85422580660841	-22.07739630215031	5.41414847791819
H	29.83767765539232	-23.23455276325670	6.27527036720796
H	30.92135061398818	-24.59733149992891	1.70838143336503
H	29.91536407992491	-25.84888775029583	2.44012810824405
H	29.58201738983788	-24.14354649069923	2.76828265535815
H	33.46618166291012	-27.69567106484191	0.13043423523565
H	34.12480778533834	-29.33057540876379	0.00195992220103
H	32.60326457698551	-29.05081985812138	0.85929899873283
H	35.98080131183757	-30.25543318680898	0.63643873827956
H	37.41678665381489	-29.63359184211372	1.45863994648137

H	36.49666312813591	-30.95712690217929	2.17468211169263
H	33.79514909671686	-22.48233944781179	10.72059550931611
H	32.32905512624587	-22.96181808976212	9.85607119326587
H	33.43789825736553	-21.79594328925733	9.13078191604969
H	37.05108431157088	-23.85765452956030	10.57714602848998
H	36.19802377426314	-25.19803434933706	11.34478106102697
H	40.08220194908360	-28.74729895479465	8.68299462216748
H	39.69325306227442	-27.06032434833789	9.04467154966316
H	38.73393270718768	-28.35891230689518	9.75746461909861
H	38.99235904112711	-30.69347499801434	5.84698233964768
H	39.94400463392668	-29.39263040615510	5.12552977524435
H	40.21256903785993	-29.85298393902713	6.81132272598665
H	35.54336002252467	-23.55966771474011	11.45181149966238
H	31.61641558994124	-31.88684190815405	5.70079287767286
H	32.80296130645021	-33.20109933242644	5.59535247314852
H	32.85938176740554	-32.06389841142304	6.95460671076318
H	34.64041261765360	-31.47365346881850	5.31874451796792
H	33.43481745782281	-31.34660850688342	4.01855555747988
H	32.29145379345047	-26.62360631151799	7.59663290807266
H	31.66869674434947	-28.17206695351568	6.98414725194785
H	32.70416949773990	-28.14913470559705	8.40903270076409
H	32.21978189461677	-26.79960605725887	2.09646402209703
H	37.32337252478398	-26.25350114467309	9.45240513781519
H	37.63691555563172	-29.54739739583890	4.01556442519429
H	32.11472202350836	-23.23617609600378	7.37382135837222
S	35.98557409551975	-24.66039537150546	4.76342092589941
C	37.41699995591246	-25.30419907368792	3.81298181818975
H	38.13055322738019	-25.83085615015391	4.45754407643206
H	37.10076078999522	-25.99315934258042	3.02100109342662
H	37.94062565288083	-24.46260623583526	3.34304368909480

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B3LYP Scan/Thiolate IPC Model/RKS/280 degrees Constrained Optimization

C	30.39024506165862	-24.81939857823565	2.59937849345053
C	36.03149681763926	-24.28665940359172	10.77731870397236
C	39.36425639912132	-29.77802160647496	6.05584182650499
C	33.58127451331571	-28.61081705601396	0.64953918565044
N	33.08065327864963	-25.55989641403968	5.11353273237271
N	34.69707279286409	-25.40471785183960	7.45007823898512
N	34.85624449106832	-27.56328810303274	4.02249018845377
C	32.82370965115801	-26.69991174246550	2.96185459701989
C	32.74737261654184	-24.00728929063785	6.97300384045652
C	36.67325282943324	-26.33965336127336	8.55222597407428
C	36.90430223301708	-28.83726792732963	4.42381035483995
C	30.35443017955590	-22.98498101919021	5.28544275293213
C	33.39915667404495	-22.70173176912186	9.71135224946979
C	39.18482484925151	-28.12112337425332	8.85194922514159
C	36.36256308930174	-30.00519486472356	1.59799047549336
C	32.43944208156436	-25.77472805150098	3.92677658609512
C	33.81608401337704	-24.41138418925881	7.76869810183236
C	37.08534193080008	-27.22628602826707	7.56295630051248
C	35.80895937993174	-28.46563326482063	3.64784321107657
C	31.30614077055122	-24.86914824967798	3.78688649753174
C	34.14811312250828	-23.82809914393398	9.06213393884194
C	38.26962566547562	-28.06961174700243	7.66419189466397
C	35.51049156493104	-29.00872059160024	2.32900144711652
C	31.29041787336583	-24.09721518519380	4.91603778047430
C	35.25414123929776	-24.49585862717850	9.51133661767424
C	38.34542527857617	-28.76704878436443	6.49071336856099
C	34.34346931261143	-28.41699753299743	1.92726223393198
C	32.41027591250617	-24.54536590742663	5.73337988954385
C	35.58533636474601	-25.47555254054768	8.48429401891709
C	37.20278284137680	-28.34593454394325	5.69103284602013
C	33.95233086254265	-27.51276770517563	3.00072308217067
N	36.46256376406890	-27.41549886768507	6.36264779063017
Fe	34.72681063141870	-26.55255176119406	5.77400953874951
C	33.85313915924092	-31.29050094850251	5.22593724063755
C	32.82739537573195	-32.18217768388343	5.91102111234971

C	32.49878311121521	-27.62734659354542	7.41291077115539
C	33.71641526145795	-27.83657652745923	6.55453774885916
C	34.03473516819239	-29.28866956359376	6.51093356858891
O	34.62173341282217	-29.89337954430012	7.38388731450151
O	33.54119481211427	-29.89684840215062	5.39668596093029
H	29.57224783339334	-22.84853469185033	4.53021060864077
H	30.88261948401055	-22.02650207700731	5.38587692933267
H	29.85224241824249	-23.17288391504133	6.24495241472893
H	30.92884106784149	-24.54498879302740	1.68150892176881
H	29.91223392868371	-25.79064380697684	2.40864365492103
H	29.59059073821520	-24.08365776748711	2.73955096866195
H	33.45039720595366	-27.66495046878791	0.10592118607373
H	34.09656113814534	-29.30470868926095	-0.02385431693158
H	32.57507622728420	-29.01476988486195	0.83022143826107
H	35.94124215663257	-30.25016171282481	0.61655924335521
H	37.38045956506966	-29.62585923179451	1.43135073331223
H	36.46380582547727	-30.94761781090298	2.15455589392892
H	33.80477874922657	-22.46873653278998	10.70223459742570
H	32.33381278326988	-22.93901381559731	9.84087969480317
H	33.44941914330791	-21.78170806415135	9.11218434892491
H	37.04074193590407	-23.89965812984209	10.57764363151190
H	36.15577319396898	-25.22271508788622	11.33916152677632
H	40.00587210881123	-28.82938024881182	8.69547590532585
H	39.63303615796232	-27.14096536158353	9.06679395028712
H	38.65246433702831	-28.43398283704883	9.76105089663424
H	38.90356905726273	-30.75341306854607	5.84507611303352
H	39.88375754394804	-29.46593897735643	5.13892366409603
H	40.12803988659984	-29.93804829889605	6.82508818162468
H	35.53276444395809	-23.57175573233152	11.44118682446044
H	31.81753050553691	-31.95157893794559	5.55970694826029
H	33.03131046773845	-33.23740393574539	5.69624412149686
H	32.86091145040503	-32.04038792016863	6.99288032103306
H	34.85608700920945	-31.47920730812122	5.61201434843975
H	33.85238613383669	-31.43821563006372	4.14436072966202
H	32.23298493867419	-26.58026152281732	7.52825470990101
H	31.63556999691044	-28.16462973872691	6.98915254805951
H	32.67353534043077	-28.06178972561664	8.40821457223930
H	32.20538019661409	-26.76372564074543	2.07111782761306
H	37.28130663366041	-26.29204680904422	9.45087925739143
H	37.58464994295534	-29.57236724250529	4.00376555271176
H	32.12761478524681	-23.19822792393200	7.34811433652197
S	35.98589471343860	-24.66798819505238	4.74432787408209
C	37.43659671041828	-25.32549887865894	3.83301431564044
H	38.13438214236516	-25.84724931903783	4.49847516194961
H	37.13611315043396	-26.02192669847671	3.04143531958577
H	37.97288124988076	-24.49032532124948	3.36591175027092

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B3LYP Scan/Thiolate IPC Model/RKS/290 degrees Constrained Optimization

C	30.36947120448490	-24.70021104615555	2.57597739452085
C	36.00563830224304	-24.37444158833773	10.76837413482289
C	39.25842104071759	-29.85097137062220	5.97660952648376
C	33.47886416472858	-28.54353236700649	0.59688676665999
N	33.04681035844099	-25.51599549060667	5.08076344029216
N	34.66490130524517	-25.41572105599181	7.41956664899296
N	34.77935218980586	-27.54501479744095	3.97484951339930
C	32.75573600467818	-26.64375560686567	2.92791634839188
C	32.75543218843714	-23.96286450577273	6.94704516596506
C	36.60491820733853	-26.42002259038807	8.52536966784169
C	36.81721381761482	-28.84333634486966	4.35042458982176
C	30.39573949995362	-22.86364119848555	5.26154953643020
C	33.42362019976319	-22.70639239660493	9.70321693876361
C	39.07841467933742	-28.25673638440832	8.80987071806625
C	36.25456240525120	-29.96627198272756	1.51069649623202
C	32.39647400652598	-25.71142308448979	3.89605291161529
C	33.80760046695308	-24.40453614228580	7.74431210528144
C	37.00083897900959	-27.30607599049823	7.52797570861517
C	35.72507199813696	-28.44737672798241	3.58311433895203

C	31.28780164643682	-24.77524887742824	3.76011661270420
C	34.14773770255714	-23.84433083805241	9.04603328748838
C	38.17098249354691	-28.16862797899342	7.61834268404524
C	35.41739911571231	-28.96922172901252	2.25758067856344
C	31.29827622204797	-24.00229122791952	4.88884781170116
C	35.23173652707396	-24.54711582333641	9.49490897300604
C	38.24473960880810	-28.84225456627452	6.42969925278699
C	33.25187882167224	-28.36688749220546	1.87029041746563
C	32.40716347800166	-24.48244231360810	5.70257191579042
C	35.54273964679691	-25.52494569292044	8.45947642449456
C	37.11238366402237	-28.39008426585377	5.63296839352134
C	33.87207103817091	-27.47356126671185	2.95715271163067
N	36.37885865705766	-27.46590990710274	6.32264943135346
Fe	34.66643324299259	-26.55253761329707	5.73741670702832
C	34.40858620743385	-31.33884927568947	5.67427095807247
C	33.28497598271603	-32.28673351907624	6.06892910096953
C	32.32389034238642	-27.58962734141935	7.23591671499244
C	33.63307948545874	-27.81227624140324	6.52971407513062
C	34.05350539589777	-29.22769412934605	6.72077331851537
O	34.42705585169898	-29.68412592618050	7.78281743452827
O	33.94326342404987	-29.98052161559639	5.59463226868803
H	29.61355449529031	-22.70664160241601	4.51043713740712
H	30.95109304144072	-21.92019748540815	5.35745942572437
H	29.89386127186230	-23.03603180171564	6.22407515836356
H	30.90979394696832	-24.42912960503220	1.65810382475334
H	29.87341105584296	-25.66134251902960	2.38031280202391
H	29.58332967283998	-23.95147602008922	2.72382903182042
H	33.33733256088750	-27.58947827628786	0.07071269870189
H	33.99157106714578	-29.22310499610369	-0.09281570037044
H	32.47675412536898	-28.95673875685243	0.78017344574431
H	35.83836831724346	-30.17675845048330	0.51916918837957
H	37.28274312458025	-29.60702150087901	1.36446782126992
H	36.32756516713879	-30.92558408062447	2.04291139169154
H	33.84460503259115	-22.47861685844407	10.68886669249424
H	32.35638071872737	-22.92767247997960	9.84569440012704
H	33.48041751997478	-21.78798182446881	9.10231628831626
H	37.03523342368612	-24.04030829415529	10.57744593707606
H	36.07650818324068	-25.31396663193861	11.33383148079055
H	39.89177552029948	-28.97175616256860	8.64410086826621
H	39.53752336701216	-27.28692526846654	9.04735043218438
H	38.53588528252453	-28.58105892157182	9.70880226348227
H	38.79188771568255	-30.81437117998534	5.72709892514476
H	39.79396775747155	-29.51497399502939	5.07752919810513
H	40.00943156340757	-30.04391659527357	6.75077890848292
H	35.53765000246975	-23.63285364473087	11.42526720072380
H	32.43536116851230	-32.18408892366340	5.38783249440197
H	33.63001662983449	-33.32637046759634	6.03253414134373
H	32.94409594772153	-32.07456547166650	7.08448829360515
H	35.23371019055225	-31.39145367481600	6.38587449131491
H	34.78360553168195	-31.56025299221493	4.67313743401112
H	32.00782308332662	-26.55053382879110	7.23254010063078
H	31.53114958855597	-28.19410894931591	6.76607855018878
H	32.40319254560664	-27.94055759577169	8.27433735364306
H	32.13313641065908	-26.69172050996659	2.03913461057227
H	37.20767767371461	-26.39891037636804	9.42856974112894
H	37.49357833515889	-29.57267349157829	3.91389486082243
H	32.15734787710431	-23.13993883817009	7.32703660499554
S	35.95744264186205	-24.68940247047293	4.70145038700490
C	37.47682898037887	-25.34704532748660	3.90961797832584
H	38.12792429086574	-25.85350255408338	4.63168331192456
H	37.24076056219192	-26.05678913994921	3.10798883698838
H	38.03955172036931	-24.51385022358670	3.47091527076959

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B3LYP Scan/Thiolate IPC Model/RKS/300 degrees Constrained Optimization

C	30.34944223919994	-24.71059445940418	2.58341962988220
C	35.99923714163065	-24.39577487293531	10.76682645558907
C	39.25719769168986	-29.84716880577242	5.95654053051433

C	33.46340113401777	-28.54345966711085	0.59105350646686
N	33.04040054654180	-25.51710630638671	5.07587288053329
N	34.65658563247097	-25.42556153453807	7.41521731380787
N	34.76228107803762	-27.55422703954586	3.97261666031770
C	32.73526179012561	-26.65543371505199	2.93077915009272
C	32.76632330974439	-23.95105925961751	6.93398814827140
C	36.58096819179720	-26.45179526924171	8.52910531663050
C	36.80995916216508	-28.84140621931449	4.33598565618705
C	30.40280866507716	-22.85160315220018	5.25371782084707
C	33.44469847169503	-22.69458858470385	9.68842999607172
C	39.05886212316700	-28.28468559036344	8.80633157607282
C	36.25405359519843	-29.94599731483487	1.48971424497330
C	32.38233138560608	-25.71823220049661	3.89659553125464
C	33.81244740022834	-24.40170628336453	7.73434922022861
C	36.97591288958687	-27.33730101433098	7.53062266847502
C	35.71482673638824	-28.44619341820009	3.57318773879861
C	31.27664373413674	-24.77842374926245	3.76096948158953
C	34.15567602615945	-23.84344659560513	9.03602987411858
C	38.15062280273514	-28.19398464358469	7.61546397647487
C	35.40924973164761	-28.96164532741520	2.24473164476129
C	31.29845525453188	-23.99636575730782	4.88322132713901
C	35.22748713043355	-24.56089007253000	9.49104031569580
C	38.23169526973470	-28.85491136137070	6.41974690544063
C	34.23736880792861	-28.36789425200938	1.86398739043954
C	32.41000841365705	-24.47559610830340	5.69389231734038
C	35.52893540062055	-25.54506839293240	8.45887311340580
C	37.09752594179020	-28.40342498657986	5.62540871579847
C	33.85329135463193	-27.48319805937081	2.95667630054085
N	36.35522684774908	-27.49244244492001	6.32340833791286
Fe	34.64873065951669	-26.56605445831093	5.73576506154905
C	34.50933228459436	-31.32066824455828	5.74897368791103
C	33.35623079207389	-32.27642262856951	6.01952660348210
C	32.31624201279408	-27.54300927613762	7.27700630289348
C	33.60076974909310	-27.80803154293343	6.54006421793324
C	34.00211292182131	-29.22584527456480	6.76119531638283
O	34.23007849226835	-29.69955848108525	7.85810596239036
O	34.05075806878443	-29.96395166371759	5.62325961148275
H	29.61729926126760	-22.69594988283005	4.50585064697938
H	30.96260109120745	-21.90998418647271	5.34108159665863
H	29.90541665196791	-23.01637173459802	6.21988433481849
H	30.88450322363857	-24.45711328615686	1.65750605268334
H	29.84306952118493	-25.66974831852367	2.40504860931589
H	29.57132166868632	-23.95281918460833	2.72743890261610
H	33.31778632697906	-27.58852102825315	0.06760045280044
H	33.97774183874404	-29.21934226449360	-0.10104900445057
H	32.46306160563481	-28.96084083403357	0.77446839268419
H	35.83637023224669	-30.15613339507492	0.49874724268933
H	37.27779981658915	-29.57511805597173	1.34132792702744
H	36.33918918050034	-30.90702239757618	2.01695428955263
H	33.86075579223021	-22.47495746997281	10.67800520704325
H	32.37294332443476	-22.89910787309861	9.82135618624832
H	33.52137216075866	-21.77635538154772	9.08942651727762
H	37.03094729964761	-24.06595700099601	10.57942642925035
H	36.06409662333038	-25.33734572335005	11.32943235222845
H	39.87677354042811	-28.99330372869806	8.63553470510480
H	39.51198214531154	-27.31362420227734	9.05007937815629
H	38.51881969756819	-28.61826997864515	9.70337739510562
H	38.80259513865223	-30.81307597037238	5.69507285249324
H	39.78950141804109	-29.49413976464838	5.06210626713054
H	40.00981759900537	-30.04004941824027	6.72917020857131
H	35.53345759980149	-23.65390113601385	11.42497424546953
H	32.57901055441778	-32.16882602478943	5.25746755853956
H	33.70842362075785	-33.31428135405340	6.00559772381240
H	32.91505437444403	-32.07674138980376	6.99816804843881
H	35.25639255996024	-31.37173962952202	6.54246201355673
H	34.98810348173509	-31.53624037514271	4.79190776362619
H	32.01289675477952	-26.50119411028219	7.24588109479940
H	31.49937991450065	-28.15402715520574	6.85954211446874

H	32.42834291417000	-27.85748437898764	8.32320374600751
H	32.10931112804438	-26.70540652585666	2.04447576696383
H	37.18170965007270	-26.43535101561882	9.43375020788575
H	37.49389102499480	-29.55848840667972	3.89096799408876
H	32.17707570046129	-23.12003733479285	7.31004802025241
S	35.95762662348700	-24.70824219014927	4.70665909362017
C	37.47734352998358	-25.36342038373879	3.91371270696130
H	38.12660962315658	-25.87504914411995	4.63383260411923
H	37.24169885740530	-26.06843255088420	3.10781732934684
H	38.04195273370032	-24.52853788543617	3.48069892236057

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B3LYP Scan/Thiolate IPC Model/RKS/310 degrees Constrained Optimization

C	30.33397415960644	-24.70137651759766	2.58845798601916
C	35.98734435247572	-24.42700733760246	10.77023428516991
C	39.25096433428001	-29.84021670779618	5.92727458668401
C	33.41692004565725	-28.56372332509952	0.60000220243362
N	33.02852441959936	-25.51706228411492	5.07372688417211
N	34.64671872666638	-25.43571814968229	7.41158163207874
N	34.73627514410841	-27.56209973412556	3.96994588229931
C	32.70145621494656	-26.66879015048980	2.93927590098035
C	32.77916618169859	-23.93527921758396	6.92199098713235
C	36.55414823376869	-26.48616646033017	8.53249649915180
C	36.79949193263128	-28.82981787709380	4.31448620380615
C	30.42615737822782	-22.81664332890667	5.23975410215649
C	33.46605171661445	-22.68487697539831	9.67684046038540
C	39.03282588208975	-28.32060455979567	8.79920698423298
C	36.22720713884782	-29.94178308477959	1.47575762758940
C	32.36196853751809	-25.72111352660319	3.89985970318347
C	33.81658310373911	-24.39901739383411	7.72617126446569
C	36.95041955602896	-27.36557361497715	7.52876683831664
C	35.69498279920882	-28.44317244170633	3.56126004139102
C	31.26678809531141	-24.76944772531095	3.76150079344326
C	34.16253363350568	-23.84503869193570	9.02883683411930
C	38.12823822090554	-28.21836629914712	7.60640297469917
C	35.38264100668066	-28.96096414443119	2.23531474362132
C	31.30489254795994	-23.97654888159196	4.87573533043966
C	35.21989149508443	-24.57968297433797	9.49030579379322
C	38.21756157682908	-28.86106600091615	6.40091589458188
C	34.20130359821734	-28.37939556231919	1.86530650150803
C	32.41393902731853	-24.46251768050188	5.68561606554236
C	35.51184077259434	-25.56835871628666	8.45978501272383
C	37.08295016517796	-28.40577922463803	5.60945518228813
C	33.81952879343623	-27.49682581212796	2.96074264470455
N	36.33205507558090	-27.51084814419330	6.31870510939151
Fe	34.62767108918370	-26.57775531087001	5.73413463224600
C	34.65527938871095	-31.29407444825480	5.86414769658404
C	33.48885193252801	-32.26888989593375	5.94062417409523
C	32.29464091013706	-27.50912648317267	7.29185692320148
C	33.56953287417900	-27.80695349975291	6.55019625105270
C	33.96157674560123	-29.22319698643431	6.81191149488526
O	34.02760888146317	-29.71498178782226	7.92413060477523
O	34.19945542035963	-29.94355983279734	5.68872833331721
H	29.63916173282487	-22.65763753968425	4.49420351223827
H	30.99881958437782	-21.88180861196509	5.31557583997892
H	29.93131431979582	-22.96591493179567	6.20969567275034
H	30.86705752703318	-24.46428157087093	1.65709318068087
H	29.81409867366453	-25.65556986549398	2.42273608921616
H	29.56650840933798	-23.93218938907053	2.72906282103653
H	33.25888781172367	-27.61096321925288	0.07613657510959
H	33.93033580618189	-29.23683497304214	-0.09546378499718
H	32.42166290177241	-28.98866913310115	0.79329459313534
H	35.80480758885928	-30.15416555537164	0.48725246029660
H	37.24866248527087	-29.56709167722682	1.32144802376972
H	36.31853097863777	-30.90198347065704	2.00348443207010
H	33.88562329861765	-22.46604959711481	10.66508656555937
H	32.39200480634454	-22.87585520538586	9.81141855232744
H	33.55341021834410	-21.77037751298196	9.07365933644004

H	37.02790954880145	-24.12345614548675	10.58758434297199
H	36.02581592097262	-25.36704966483592	11.33785379079400
H	39.85165165817310	-29.02708113705846	8.62402748805065
H	39.48467234195691	-27.35181443589998	9.05411810205056
H	38.49021942995960	-28.66316175423644	9.69133707206434
H	38.80350172191375	-30.80490961574145	5.64947331491973
H	39.78447072609119	-29.47027055902867	5.04047543670748
H	40.00163342686302	-30.04000903898730	6.70003811752751
H	35.53575374116799	-23.67064468143799	11.42172522057111
H	32.84175914956252	-32.16728270847364	5.06482454575576
H	33.85441450138070	-33.30145919328011	5.97971958318557
H	32.89418588410678	-32.08149778625246	6.83708036433993
H	35.27096003201251	-31.35016084913621	6.76311353749660
H	35.27934872351674	-31.48666851792059	4.98951544548674
H	32.00819185934771	-26.46357323575563	7.24610974404105
H	31.46445612970827	-28.11173751083001	6.88869237634307
H	32.40706194774615	-27.81219092216262	8.34050799035245
H	32.06926670229622	-26.72148312436970	2.05755251314130
H	37.15099247194338	-26.47821684128891	9.43981995655171
H	37.49024862547674	-29.53440520005913	3.86007415572258
H	32.20146346100818	-23.09449239899354	7.29412612655623
S	35.94600387659055	-24.72352061008522	4.70145411529795
C	37.47895875872052	-25.37052830019435	3.92787952039488
H	38.12105483286167	-25.87970660050935	4.65614864653311
H	37.25739362768276	-26.07635293126257	3.11865412505791
H	38.04525033387270	-24.53279329340435	3.50268184181167

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B3LYP Scan/Thiolate IPC Model/RKS/320 degrees Constrained Optimization

C	30.31717580186556	-24.72089056892512	2.60112204782510
C	35.98199181202725	-24.44340768506468	10.77388629442981
C	39.26025649558098	-29.82683541552749	5.91660551131422
C	33.40919079934867	-28.57259087620910	0.60357744429126
N	33.02500133327309	-25.52470750467381	5.07562426748245
N	34.64440289167162	-25.44295732074635	7.41145838260565
N	34.72853156935960	-27.57008849118750	3.9732877439877
C	32.68584897723697	-26.68762772676993	2.94931757116579
C	32.79138863492754	-23.92785572137248	6.91330885786418
C	36.53909434222812	-26.50789118854022	8.54043321384565
C	36.80584530376208	-28.81831285281175	4.30597565869198
C	30.43362261645901	-22.81370675964982	5.23560137259702
C	33.48574015813009	-22.67296574279805	9.66468785564826
C	39.02052341313189	-28.33922310954289	8.80355138369156
C	36.23752724817063	-29.92293210804008	1.46485184117669
C	32.35090617094045	-25.73567245514671	3.90717774852582
C	33.82480101090481	-24.39606972102956	7.72006140336790
C	36.93840408246351	-27.38257623534133	7.53354572500818
C	35.69595762983254	-28.43865097750725	3.55757794693865
C	31.25782307752849	-24.78172144956817	3.76827012927129
C	34.17244527005906	-23.84200583077710	9.02215955427549
C	38.11958716192584	-28.23114799867938	7.60845769703507
C	35.38480848700268	-28.95426336374741	2.23074935363127
C	31.30637715973169	-23.97923983880407	4.87517883828405
C	35.21874430348338	-24.58821951678064	9.49046194001102
C	38.21802860684058	-28.86004680855048	6.39633609618797
C	34.19536368314194	-28.38499509539050	1.86726861097026
C	32.41831429995896	-24.46269496739662	5.68251724573392
C	35.50391940906590	-25.58236497395540	8.46344787903376
C	37.08376465259290	-28.40345163738623	5.60498085960696
C	33.80844399045594	-27.50988850827076	2.96684508621868
N	36.32491361032663	-27.52045950999488	6.32017751843589
Fe	34.61874592144692	-26.58897778084630	5.73583006116742
C	34.70307303314429	-31.28446460023206	5.91032364770849
C	33.51814822991764	-32.24041353736333	5.88229987023481
C	32.30625427009811	-27.47405574996655	7.33640538021291
C	33.55379155323421	-27.80885708099845	6.56290756274686
C	33.90916502325997	-29.23740022453866	6.82478594503673
O	33.82057497165687	-29.77640233169654	7.91526245856644

O	34.29124360454230	-29.92273956443391	5.72058817648269
H	29.64456617824961	-22.65592391322681	4.49201559499785
H	31.01031555566090	-21.88079278344913	5.30381790232758
H	29.94179505832504	-22.95546433425558	6.20817983879947
H	30.84434464643437	-24.49300987540198	1.66409499424521
H	29.79373514577716	-25.67506963024782	2.44709635772981
H	29.55264665899048	-23.94860099931411	2.74059404744912
H	33.24046529087162	-27.61957581506754	0.08354548240602
H	33.92731084107857	-29.23825741226254	-0.09555239960873
H	32.41870206153804	-29.00798817126289	0.79801088585724
H	35.81887459851107	-30.12956878836713	0.47354191168722
H	37.25665850537498	-29.53982978949459	1.31623634026074
H	36.33415780599028	-30.88698665033651	1.98459314887852
H	33.91698499849301	-22.44408088107113	10.64558850819409
H	32.41277946925412	-22.85980140607079	9.81350413878068
H	33.56849746695899	-21.76588765569437	9.04995976447965
H	37.03320088571582	-24.17747580653461	10.59419962457294
H	35.98569532520666	-25.37631496875881	11.35467577457089
H	39.83770097216281	-29.04770401469899	8.62877680250486
H	39.47464140573086	-27.37247039959265	9.06231630993153
H	38.47467827779490	-28.68240780125938	9.69346862746159
H	38.82024264736000	-30.78964147459561	5.62115645181532
H	39.79857881797751	-29.44080886127947	5.03960722416250
H	40.00601940684557	-30.03392458632159	6.69219870761064
H	35.55148262077879	-23.66351641891247	11.41173026310892
H	32.94629471800005	-32.11775921240196	4.95818832247942
H	33.86376015374753	-33.27911235613605	5.93784565474189
H	32.85741800443063	-32.05184044697207	6.73019148130993
H	35.24848891689002	-31.36716025786452	6.85211379610748
H	35.38747368661051	-31.47681115945945	5.08195520326255
H	32.04156858939848	-26.42342594320455	7.28708940223272
H	31.45192695910280	-28.06185918438474	6.96325904301816
H	32.43706581074868	-27.77072232809196	8.38402275266921
H	32.04961716991912	-26.74464455111749	2.07079687403936
H	37.13205734991040	-26.50499571484966	9.45032893577875
H	37.50329787376864	-29.51252906870746	3.84582980054211
H	32.22029782765639	-23.08058292040105	7.28081988291241
S	35.94542985982881	-24.73253258936122	4.70529022055028
C	37.46518910176967	-25.37584608471841	3.90393178400281
H	38.11512471376296	-25.89490081090419	4.61821364932934
H	37.23004610870460	-26.07288887488871	3.09098840419206
H	38.02861458893889	-24.53579332879805	3.47958668488705

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B3LYP Scan/Thiolate IPC Model/RKS/330 degrees Constrained Optimization

C	30.30710362282324	-24.72633908884287	2.61573516122552
C	35.98051346930200	-24.45766793928102	10.78131980949687
C	39.27751386147418	-29.79738533639098	5.89544125033326
C	33.36908559180014	-28.60664750438063	0.63026160879895
N	33.01846734029345	-25.53295070288149	5.08542454828964
N	34.64301851384621	-25.45075654507070	7.41703711344969
N	34.70657651019960	-27.59173191620996	3.98900425309314
C	32.65705556611311	-26.71466833651516	2.97352612245183
C	32.80848112898823	-23.91651994582116	6.90882366376275
C	36.52975562194896	-26.52550016703283	8.54912807786310
C	36.80267393607075	-28.81247905923529	4.30195765002141
C	30.46199965558893	-22.78815401154965	5.22569417794965
C	33.50826567863411	-22.66143784112246	9.65841739375989
C	39.02473381544733	-28.34034017474661	8.79630593180962
C	36.21840233000346	-29.92828340600847	1.46705661650985
C	32.33569980036852	-25.74993090269583	3.92318638498491
C	33.83437520434298	-24.39349124446195	7.71980022486908
C	36.93125198316394	-27.39379497953698	7.53723694594390
C	35.68017355620820	-28.44941482012991	3.56452871121702
C	31.25308205444910	-24.78486501270228	3.77865460741154
C	34.18425360768592	-23.83961563295770	9.02124934673276
C	38.12036734490952	-28.23218423145950	7.60378288822085
C	35.36227713476975	-28.96890366610116	2.24087157891788

C	31.31771968894409	-23.96930671788402	4.87513836508309
C	35.22010954721951	-24.59664150915583	9.49555828657972
C	38.22413172108149	-28.84783974348756	6.38536268017858
C	34.16349286803308	-28.41232790635693	1.88785460353973
C	32.42723783599411	-24.45704143159473	5.68303840095656
C	35.49857076189005	-25.59563876958054	8.47157009060126
C	37.08268846827803	-28.39774109715511	5.60053768915515
C	33.77868933646385	-27.53858057700610	2.98927440733198
N	36.31696440538005	-27.52791729910575	6.32422091496017
Fe	34.60751620153230	-26.60462065920956	5.74831640975167
C	34.77175535394311	-31.27810490886461	6.01828760571757
C	33.60662041271387	-32.21214601419788	5.71899533161530
C	32.28681995235738	-27.44403201382372	7.34891935159899
C	33.53198261338228	-27.81409785234801	6.58595781596392
C	33.83211628330239	-29.25746525874477	6.85072076679979
O	33.55004668247662	-29.84148008600334	7.88565270060426
O	34.41551747674629	-29.90449803610955	5.81405936860085
H	29.67343837735793	-22.62686841528000	4.48237909269937
H	31.05192358251697	-21.86286074220554	5.28313826806109
H	29.97058408127603	-22.91336186175552	6.20072899428700
H	30.83230666858428	-24.51873572959082	1.67293624994042
H	29.76919778100623	-25.67489264852274	2.47758958543505
H	29.55436954045989	-23.94144178082807	2.74877606926167
H	33.19438069014245	-27.65592820349556	0.10792221961197
H	33.88418385087461	-29.27352894873636	-0.06991053881960
H	32.38107022513214	-29.04374059276526	0.83296516741698
H	35.79326110931667	-30.13873494174135	0.47929466554182
H	37.23197133909193	-29.53416561509244	1.30961347793459
H	36.32973422613127	-30.89134430016940	1.98551455354504
H	33.94051102124741	-22.43308337360146	10.63899141331223
H	32.43336486806569	-22.83727956379283	9.80643764112621
H	33.60071384997529	-21.75759040748634	9.04033089394506
H	37.03628173916749	-24.20835362615501	10.60459830410677
H	35.96806761165031	-25.38806055254918	11.36605640017477
H	39.84440818271115	-29.04488435374628	8.61737669469482
H	39.47544075406483	-27.37253682695925	9.05719667833790
H	38.48275710734170	-28.68855099848157	9.68666568927259
H	38.85059164096804	-30.76502750866875	5.59648846272861
H	39.80619819992403	-29.39854631824601	5.01835700245176
H	40.02969816038098	-29.99799277133051	6.66651740168856
H	35.55933624910655	-23.66868793823057	11.41418577744089
H	33.22329374840031	-32.03700888107118	4.70996395981098
H	33.92754949972301	-33.25794828983596	5.78847067987033
H	32.79676687223228	-32.05344989144727	6.43334237053305
H	35.12373926836490	-31.41191243089115	7.04288496528454
H	35.60088487644162	-31.44585792499877	5.32793252380683
H	32.03576382697931	-26.39222691149180	7.27399924150753
H	31.42540650108413	-28.03099955872440	6.99307397499589
H	32.40994326712735	-27.71546417669388	8.40411677913395
H	32.01517089894189	-26.77597518244680	2.09942273248689
H	37.12263468925092	-26.52543024641323	9.45908874883152
H	37.50667081763032	-29.49542775559388	3.83484460968135
H	32.24787728946188	-23.05975159644399	7.27030635305702
S	35.92998434491876	-24.75098085195614	4.69968101436187
C	37.45284453375308	-25.38603133961183	3.89854461486636
H	38.10526980461252	-25.90163684903245	4.61307832615927
H	37.22095814903862	-26.08506469611294	3.08635661680170
H	38.01183050237287	-24.54337315204044	3.47354787446375

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B3LYP Scan/Thiolate IPC Model/RKS/340 degrees Constrained Optimization

C	30.28806849351138	-24.76817208115909	2.64319433840809
C	35.98885548573386	-24.44361176690083	10.78582558133829
C	39.29599521898481	-29.77822495800223	5.90694894865019
C	33.35597464554680	-28.64751514422082	0.66413804171330
N	33.02026722748468	-25.54404342755975	5.09926896538510
N	34.65023730047142	-25.44731834915767	7.42512445767035
N	34.70203558342308	-27.61085161400505	4.01293454765990

C	32.64326966045969	-26.74935944913996	3.00334706770035
C	32.82441890842789	-23.90692852770205	6.90596207876169
C	36.53108543221091	-26.52465147533274	8.56389296284782
C	36.81189986947798	-28.81028053406657	4.31695723173693
C	30.46744005327588	-22.79572028409293	5.22612164881855
C	33.53136457102350	-22.63680718120623	9.64795691742119
C	39.03179221768962	-28.33094964535102	8.81122394854964
C	36.22458658303454	-29.93682259955893	1.48731565183832
C	32.32797086602208	-25.77521674930674	3.94532635551322
C	33.84898857050137	-24.38208923323278	7.71976127507599
C	36.93381888993815	-27.39289431617575	7.55249748134949
C	35.68191702689842	-28.46021142817036	3.58500082401084
C	31.24462690330150	-24.81139595309235	3.79805614802972
C	34.20048748388298	-23.82291608751968	9.01837774544638
C	38.12729048866761	-28.22563233770326	7.61850239287818
C	35.36145671546729	-28.98651420040062	2.26486192835007
C	31.31939427981322	-23.98182094908374	4.88328431731770
C	35.22965902487067	-24.58486151378760	9.49956554894474
C	38.23561654241329	-28.83735763371917	6.39877558264512
C	34.15457490977262	-28.44323563262553	1.91756156978349
C	32.43474610544314	-24.46046745355645	5.68861672329616
C	35.50332971001940	-25.59136250122293	8.48172892732249
C	37.09143063241677	-28.39255692800518	5.61452227003472
C	33.76859944009988	-27.56871499588320	3.01799394717591
N	36.32118061499413	-27.52781431805032	6.33911091869510
Fe	34.60800646280730	-26.61281858160650	5.76486071572915
C	34.75345336911204	-31.27781147471524	6.01970658853450
C	33.62428027475045	-32.14807292594316	5.48267587011624
C	32.31721638638672	-27.40709620437010	7.42000040755041
C	33.52574993929544	-27.81201264813162	6.61531936871670
C	33.75258939281508	-29.27795547350826	6.83005895359805
O	33.30822703355690	-29.91484150283029	7.77411318141697
O	34.47079255378168	-29.88357639212637	5.85498477505691
H	29.67259721699960	-22.64342978125938	4.48764300599133
H	31.05845958756204	-21.87024695233819	5.2666627309079
H	29.98446719069032	-22.90841082223291	6.20684575609320
H	30.80475507495292	-24.57563982674893	1.69252421827317
H	29.74730399887315	-25.71769771381015	2.52425781926709
H	29.53791441546280	-23.98004881666024	2.77148764848913
H	33.17492170913655	-27.70014934316877	0.13787419231490
H	33.87158346297538	-29.31543147498230	-0.03466347832302
H	32.37086319609924	-29.08819530723475	0.87276211661379
H	35.79253058139557	-30.15970360819711	0.50531577192460
H	37.22993885796117	-29.52729294899054	1.31696335794728
H	36.35698293318360	-30.89471916690744	2.01009531756456
H	33.95707488939094	-22.41192851358748	10.63218469022481
H	32.45348521584273	-22.80148979751698	9.78640150972767
H	33.63872053440762	-21.73458949176621	9.02984806551227
H	37.04395051120956	-24.19055235982787	10.61001664462816
H	35.97921324388282	-25.37420925701029	11.37021372761497
H	39.85613211283650	-29.02965139037220	8.63086791523658
H	39.47600301007360	-27.36092322383821	9.07495947175167
H	38.49182874968763	-28.68499764435663	9.70056763501215
H	38.87699398515090	-30.74904021128667	5.60698026433636
H	39.82088061635243	-29.37394486093038	5.03007736505804
H	40.05034275770830	-29.97379256620116	6.67722624130284
H	35.56467334547744	-23.65634276656121	11.41881451460658
H	33.40363764983604	-31.88967344903105	4.44330659923277
H	33.90536644032431	-33.20685677433520	5.52147441882327
H	32.71971430762564	-32.00958074159087	6.07764280771013
H	34.93755085440804	-31.48724093610563	7.07519302639659
H	35.67431176414568	-31.43518683154969	5.45424274573714
H	32.07013710332093	-26.35665926257147	7.32145725132532
H	31.43752487583082	-28.00241338410850	7.13345240637511
H	32.48671277101467	-27.63679061347614	8.47939739600925
H	31.99539688795109	-26.82029637333909	2.13444568504163
H	37.12349282298479	-26.52332682613856	9.47417556869307
H	37.52070592682490	-29.48668556214964	3.84761746417438

H	32.26875043582961	-23.04393660471838	7.26011894477927
S	35.93388255640242	-24.76348759105835	4.71332977000061
C	37.43303059419607	-25.39945500999698	3.87040143889815
H	38.10105601123824	-25.92129933499379	4.56587535689563
H	37.17758708064589	-26.09447861590152	3.06188743279175
H	37.98431653732219	-24.55697987092573	3.43528984376916

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B3LYP Scan/Thiolate IPC Model/RKS/350 degrees Constrained Optimization

C	30.26439574015623	-24.81728363077891	2.69350453299749
C	36.02957572949565	-24.39981568010438	10.78587994829023
C	39.32157632429812	-29.75210755265283	5.92663685224574
C	33.32023986177177	-28.71833654761217	0.73317018288757
N	33.02247753614250	-25.55763522711195	5.13110718169362
N	34.66100331536268	-25.44623526624934	7.45023956623569
N	34.69538904310848	-27.63889999693648	4.05605565038855
C	32.62200590531047	-26.79710674585840	3.05930582707526
C	32.84612084339123	-23.89678693709246	6.91695465458027
C	36.54510614915726	-26.51508496691793	8.59000295782910
C	36.81954219561604	-28.81355673014585	4.34961090198214
C	30.47921433495004	-22.80105722080363	5.23964339024546
C	33.57891531591564	-22.59159377296123	9.63558587258184
C	39.05718577749226	-28.30575413597973	8.83066427480323
C	36.21391882946349	-29.97014753361163	1.53369148827784
C	32.31748916520942	-25.80724258881650	3.98856538959071
C	33.87005255237268	-24.36958847526313	7.73282959718642
C	36.94561315162844	-27.38651457958772	7.58035718406019
C	35.67854546684634	-28.48226845961038	3.62528752280297
C	31.23474698843472	-24.84315731747288	3.83732334639099
C	34.23336267487868	-23.79384932740339	9.02114925561214
C	38.14581810348671	-28.21018464029053	7.64235633351817
C	35.34758199008505	-29.02482403680154	2.31432415608258
C	31.32421365567489	-23.99506307578384	4.90717941791513
C	35.25880448011192	-24.55704966415911	9.50829275228454
C	38.25448437297146	-28.82093968631398	6.42239094067155
C	34.13045063257579	-28.49682133731029	1.97635202662514
C	32.44591609383630	-24.46403588719703	5.70912850806739
C	35.51911819336372	-25.58032064230294	8.50371759273423
C	37.10292833538114	-28.38665672146136	5.64285303388262
C	33.750164447527737	-27.61355709045092	3.07177768360093
N	36.32911402785243	-27.52692672722794	6.37040003343491
Fe	34.61121854179495	-26.62566987669821	5.80200669220568
C	34.71859395458709	-31.29004995423730	6.02507437391919
C	33.71422068596142	-32.03375288684792	5.15380177290660
C	32.28296657431395	-27.39432628318345	7.40883680204896
C	33.50372599262742	-27.81960324259632	6.63390151704086
C	33.62197239235088	-29.31022245120607	6.75260755591823
O	32.95478515608291	-29.99950516787866	7.51269670275706
O	34.54561763477095	-29.87205510738867	5.93790511862611
H	29.67798009692964	-22.65732838819882	4.50640331772742
H	31.07343509767786	-21.87698680387763	5.26074941866669
H	30.00508350104950	-22.89750374989584	6.22639073578222
H	30.77030569428000	-24.64627069484190	1.73301469858401
H	29.71708410329659	-25.76589746021645	2.60005418642403
H	29.52009087297223	-24.02265778267578	2.81551776985935
H	33.13838486446512	-27.77895511099769	0.19293640159268
H	33.82705661307341	-29.39988706589655	0.04117400944299
H	32.33536872012179	-29.15128974373672	0.95779546080110
H	35.76680840742551	-30.21653097920806	0.56412430605030
H	37.20716811059857	-29.54329821172742	1.33686396217592
H	36.37615223701138	-30.91665619872100	2.06839885545931
H	34.01573411822825	-22.35255694023922	10.61159241433754
H	32.50121440506323	-22.74553014058768	9.78704939734413
H	33.68728901340697	-21.70150056617909	9.00038705299243
H	37.08591178937451	-24.16235163530299	10.59647595179649
H	36.01480095021318	-25.31832931436979	11.38915811130321
H	39.88207564388508	-29.00378545361265	8.65020616309030
H	39.50084627735688	-27.33304735525265	9.08556917109967

H	38.52343159464378	-28.65494464302978	9.72566291830264
H	38.90982986340313	-30.72503129184832	5.62357139904812
H	39.84302920110169	-29.34095209543855	5.05087446545398
H	40.07782670037268	-29.94457347388703	6.69583888049834
H	35.61950446215567	-23.59529657838454	11.40636448223657
H	33.75330031441766	-31.66206292304665	4.12631996449905
H	33.93571490241776	-33.10731247819393	5.14469136475158
H	32.70156305368187	-31.89528602037774	5.53689805448877
H	34.63520175018398	-31.60226710310760	7.06832643199709
H	35.74053053764842	-31.45832869574332	5.67801235030926
H	32.12208021006057	-26.32317367127941	7.40108488490651
H	31.38273214444453	-27.88870112896543	7.01624607223288
H	32.36265695667603	-27.73421691734137	8.44957351401598
H	31.96351703238409	-26.88273587406965	2.19974295190058
H	37.14218461692028	-26.50671999371076	9.49723612318330
H	37.53181480281799	-29.48549656188137	3.87920803920778
H	32.29816085151515	-23.02538064999197	7.26240473114411
S	35.92079057509547	-24.78226257588666	4.71591012874456
C	37.41347151669873	-25.41566801354347	3.86051464728427
H	38.09172449531493	-25.92951907990523	4.55206118309210
H	37.15218330832491	-26.11789260265629	3.06002339312426
H	37.95527508418081	-24.57350695986553	3.41311844905119

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B3LYP Scan/Thiolate IPC Model/Trip/0 degrees Constrained Optimization

C	30.462557	-24.910081	2.334435
C	35.692491	-24.455898	10.773327
C	39.269700	-29.865183	6.146777
C	33.617823	-28.892533	0.603211
N	33.147908	-25.594713	4.864642
N	34.656585	-25.466858	7.311037
N	34.809251	-27.701329	3.957258
C	32.800089	-26.891854	2.823665
C	32.911594	-23.894694	6.612199
C	36.382838	-26.585459	8.630842
C	36.907879	-28.875758	4.409810
C	30.621219	-22.821951	4.826244
C	33.436935	-22.573781	9.368035
C	38.828354	-28.443323	9.040766
C	36.472478	-30.100276	1.599509
C	32.471289	-25.872548	3.712901
C	33.867021	-24.368660	7.508383
C	36.837522	-27.460452	7.650148
C	35.815725	-28.555200	3.611801
C	31.403191	-24.905632	3.503438
C	34.117676	-23.794971	8.823187
C	38.009073	-28.312550	7.790413
C	35.560532	-29.136100	2.300070
C	31.471700	-24.026303	4.550344
C	35.063385	-24.588241	9.417486
C	38.193555	-28.910967	6.573206
C	34.361837	-28.626870	1.878717
C	32.563393	-24.482346	5.400022
C	35.395245	-25.621738	8.449288
C	37.113068	-28.443708	5.715943
C	33.919808	-27.711465	2.921715
N	36.313001	-27.569551	6.392511
Fe	34.702373	-26.621376	5.653363
C	34.579935	-31.334352	6.047804
C	33.791020	-31.982273	4.914543
C	32.113983	-27.324859	7.122156
C	33.370074	-27.883482	6.505052
C	33.390469	-29.331901	6.561851
O	32.512370	-30.053436	7.044876
O	34.511196	-29.912152	6.009831
H	29.861565	-22.678224	4.050054
H	31.221581	-21.903020	4.871903
H	30.094328	-22.906775	5.786917

H	30.996584	-24.794121	1.381087
H	29.896554	-25.849831	2.270212
H	29.734204	-24.094642	2.401472
H	33.456665	-27.971325	0.026408
H	34.163443	-29.589979	-0.041702
H	32.626992	-29.328179	0.792442
H	36.088467	-30.368056	0.609163
H	37.476530	-29.677248	1.458728
H	36.596023	-31.033299	2.166653
H	33.810058	-22.318168	10.365825
H	32.350140	-22.714679	9.450880
H	33.596368	-21.699081	8.722669
H	36.779491	-24.309253	10.705309
H	35.530832	-25.352642	11.387549
H	39.664746	-29.136699	8.901069
H	39.251141	-27.479052	9.356081
H	38.229559	-28.818869	9.882338
H	38.856861	-30.835012	5.836207
H	39.840711	-29.474185	5.293336
H	39.982437	-30.058640	6.956136
H	35.281449	-23.604034	11.325756
H	34.110022	-31.581378	3.948600
H	33.945250	-33.068511	4.909776
H	32.725592	-31.783699	5.038738
H	34.220670	-31.695324	7.015395
H	35.646086	-31.560831	5.956217
H	32.297373	-26.399671	7.670094
H	31.379370	-27.074784	6.342196
H	31.636680	-28.049403	7.787649
H	32.178048	-27.002179	1.940733
H	36.895300	-26.599909	9.588039
H	37.637714	-29.565953	3.997323
H	32.355144	-23.010555	6.908319
S	36.126730	-25.001553	4.573168
C	37.415588	-24.481346	5.769260
H	36.974969	-24.023755	6.662255
H	38.034768	-25.327373	6.088013
H	38.065309	-23.741218	5.287645

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B3LYP Scan/Thiolate IPC Model/Trip/10 degrees Constrained Optimization

C	30.454913	-24.909420	2.335527
C	35.696633	-24.446892	10.766865
C	39.246359	-29.888261	6.152822
C	33.601284	-28.896619	0.607181
N	33.137120	-25.598035	4.868233
N	34.656607	-25.461358	7.306876
N	34.796481	-27.708135	3.960756
C	32.787028	-26.896308	2.828334
C	32.907866	-23.892078	6.610646
C	36.381224	-26.581960	8.627130
C	36.896457	-28.881398	4.410231
C	30.619140	-22.817266	4.823590
C	33.441096	-22.564829	9.361250
C	38.808476	-28.462267	9.045331
C	36.456580	-30.105404	1.598539
C	32.459744	-25.876077	3.717002
C	33.867178	-24.362971	7.504098
C	36.832409	-27.460007	7.647606
C	35.802532	-28.562338	3.613809
C	31.394227	-24.906624	3.505591
C	34.120469	-23.787259	8.817370
C	37.996478	-28.321855	7.791361
C	35.545741	-29.142017	2.301793
C	31.464888	-24.025708	4.550927
C	35.066560	-24.580349	9.411577
C	38.179591	-28.921647	6.574775
C	34.346935	-28.631595	1.881832

C	32.555498	-24.483121	5.401425
C	35.396593	-25.615310	8.444427
C	37.105173	-28.445648	5.714556
C	33.906114	-27.716886	2.925581
N	36.310642	-27.565086	6.388727
Fe	34.696895	-26.620649	5.652959
C	34.596231	-31.336123	6.099580
C	33.909333	-31.927659	4.872822
C	32.134291	-27.329823	7.170514
C	33.370436	-27.885205	6.511093
C	33.377905	-29.333689	6.532180
O	32.432127	-30.057026	6.858993
O	34.556554	-29.911744	6.115787
H	29.860925	-22.671806	4.046316
H	31.223577	-21.900932	4.867808
H	30.090939	-22.897614	5.783924
H	30.990642	-24.796531	1.382759
H	29.885629	-25.847191	2.271754
H	29.729442	-24.091241	2.400545
H	33.439815	-27.975195	0.030817
H	34.145667	-29.594254	-0.038538
H	32.610579	-29.331864	0.797859
H	36.072471	-30.368957	0.607111
H	37.461333	-29.683477	1.459851
H	36.578250	-31.040970	2.161935
H	33.815250	-22.308058	10.358355
H	32.354256	-22.704670	9.445173
H	33.600693	-21.691182	8.714491
H	36.783750	-24.301595	10.698253
H	35.534204	-25.342649	11.382368
H	39.639378	-29.162777	8.908486
H	39.238176	-27.502528	9.365130
H	38.201993	-28.834441	9.882930
H	38.823263	-30.853745	5.842517
H	39.824530	-29.505488	5.300467
H	39.954275	-30.088649	6.964710
H	35.286656	-23.593926	11.318395
H	34.317939	-31.491873	3.957437
H	34.054980	-33.014533	4.838182
H	32.839183	-31.721207	4.907830
H	34.141043	-31.727970	7.013896
H	35.662538	-31.579149	6.100701
H	32.344130	-26.422761	7.739224
H	31.385071	-27.048875	6.415445
H	31.658918	-28.065182	7.825962
H	32.164595	-27.006134	1.945636
H	36.892706	-26.597856	9.584845
H	37.623395	-29.575191	3.998674
H	32.352659	-23.006931	6.906087
S	36.116879	-25.003177	4.563887
C	37.413285	-24.487186	5.753474
H	36.978684	-24.024308	6.646693
H	38.028319	-25.336078	6.072425
H	38.065667	-23.752483	5.267207

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B3LYP Scan/Thiolate IPC Model/Trip/20 degrees Constrained Optimization

C	30.465043	-24.930021	2.311042
C	35.685771	-24.421422	10.756418
C	39.244313	-29.888406	6.183114
C	33.629980	-28.905589	0.605190
N	33.129087	-25.614061	4.864436
N	34.641803	-25.464298	7.306208
N	34.798702	-27.721109	3.970045
C	32.795173	-26.912891	2.823199
C	32.888373	-23.904245	6.601431
C	36.371347	-26.571220	8.633323
C	36.898948	-28.890579	4.429714

C	30.614015	-22.829979	4.793923
C	33.413054	-22.563397	9.345084
C	38.804851	-28.441031	9.064732
C	36.483731	-30.105688	1.611843
C	32.459945	-25.893243	3.708950
C	33.845959	-24.370210	7.498640
C	36.825723	-27.454228	7.660126
C	35.809452	-28.571911	3.627394
C	31.396516	-24.923754	3.487285
C	34.097324	-23.786023	8.807872
C	37.991746	-28.312271	7.810193
C	35.563840	-29.148883	2.312387
C	31.459859	-24.040408	4.530621
C	35.049310	-24.569821	9.405564
C	38.175907	-28.920735	6.598189
C	34.366105	-28.641419	1.885601
C	32.544447	-24.496828	5.390235
C	35.383590	-25.608477	8.443967
C	37.101189	-28.452285	5.734112
C	33.915198	-27.730916	2.928617
N	36.303636	-27.569522	6.401969
Fe	34.691275	-26.629617	5.659039
C	34.518166	-31.349131	5.992707
C	33.842744	-31.865454	4.726702
C	32.264527	-27.327898	7.393610
C	33.372460	-27.890484	6.540456
C	33.339366	-29.338606	6.497143
O	32.366982	-30.051480	6.762976
O	34.512133	-29.926051	6.078668
H	29.862871	-22.684583	4.009802
H	31.220094	-21.914896	4.841492
H	30.077510	-22.907115	5.749934
H	31.006973	-24.820458	1.361411
H	29.895974	-25.867912	2.246876
H	29.739446	-24.111393	2.368719
H	33.463395	-27.982272	0.033453
H	34.184180	-29.594360	-0.041714
H	32.642357	-29.350988	0.788079
H	36.103968	-30.372642	0.619689
H	37.485567	-29.676097	1.475536
H	36.610957	-31.039999	2.176005
H	33.788616	-22.297600	10.339311
H	32.327146	-22.708058	9.432677
H	33.566809	-21.693541	8.691860
H	36.767997	-24.245827	10.679701
H	35.553200	-25.322206	11.371529
H	39.635939	-29.142321	8.933117
H	39.234396	-27.478188	9.375298
H	38.199579	-28.805912	9.906408
H	38.821886	-30.853802	5.871728
H	39.827514	-29.507288	5.333372
H	39.947711	-30.088461	6.999021
H	35.256729	-23.581009	11.312686
H	34.282166	-31.401233	3.840470
H	33.961857	-32.953320	4.647091
H	32.777917	-31.631966	4.749303
H	34.036672	-31.773216	6.878650
H	35.578526	-31.616817	6.002055
H	32.667219	-26.942368	8.340524
H	31.763594	-26.481120	6.917469
H	31.517861	-28.090389	7.631270
H	32.179747	-27.023915	1.935814
H	36.882764	-26.578811	9.591189
H	37.629106	-29.583272	4.022084
H	32.330357	-23.019487	6.892620
S	36.102320	-25.002517	4.571126
C	37.415531	-24.506528	5.750609
H	36.993334	-24.052610	6.654419

H	38.031593	-25.361077	6.051938
H	38.064516	-23.768114	5.265372

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B3LYP Scan/Thiolate IPC Model/Trip/30 degrees Constrained Optimization

C	30.447333	-24.950574	2.326045
C	35.707971	-24.394302	10.744729
C	39.225725	-29.911704	6.202267
C	33.649538	-28.884555	0.594634
N	33.125244	-25.617056	4.869398
N	34.641446	-25.461663	7.308764
N	34.798032	-27.724667	3.974478
C	32.796163	-26.913995	2.826100
C	32.887367	-23.902947	6.602297
C	36.372232	-26.566094	8.636779
C	36.892956	-28.900316	4.440736
C	30.593305	-22.848215	4.806847
C	33.433262	-22.540805	9.331290
C	38.795235	-28.448636	9.077070
C	36.501681	-30.084077	1.604543
C	32.454553	-25.900017	3.715723
C	33.849893	-24.363699	7.497137
C	36.820184	-27.458129	7.668671
C	35.811019	-28.572899	3.631668
C	31.384347	-24.936888	3.497763
C	34.110204	-23.770239	8.800367
C	37.981513	-28.322050	7.822688
C	35.574632	-29.137521	2.309651
C	31.446246	-24.052912	4.540419
C	35.063182	-24.552200	9.398844
C	38.162267	-28.936965	6.613470
C	34.378258	-28.628617	1.880782
C	32.536995	-24.502561	5.396194
C	35.388446	-25.599881	8.443931
C	37.091133	-28.465032	5.746807
C	33.919746	-27.727819	2.928699
N	36.298095	-27.575585	6.410808
Fe	34.690177	-26.629419	5.662706
C	34.444319	-31.375337	6.015245
C	33.911889	-31.840192	4.664484
C	32.293667	-27.341698	7.447509
C	33.359585	-27.891085	6.533375
C	33.284194	-29.334053	6.425773
O	32.257881	-30.011480	6.522818
O	34.480280	-29.953992	6.139137
H	29.835310	-22.710803	4.027886
H	31.192283	-21.928081	4.847723
H	30.064342	-22.927258	5.766887
H	30.984737	-24.846502	1.373242
H	29.878640	-25.889215	2.270423
H	29.721673	-24.131896	2.382169
H	33.486769	-27.957921	0.027224
H	34.206831	-29.570250	-0.052893
H	32.660689	-29.330462	0.769554
H	36.134381	-30.332573	0.602968
H	37.505647	-29.653539	1.489135
H	36.620680	-31.029027	2.152790
H	33.811177	-22.271221	10.323612
H	32.346745	-22.679461	9.421015
H	33.590601	-21.675452	8.672935
H	36.792345	-24.236625	10.660660
H	35.564486	-25.283777	11.373846
H	39.624683	-29.152192	8.947086
H	39.227443	-27.485765	9.383934
H	38.190050	-28.809256	9.920638
H	38.798489	-30.876644	5.896203
H	39.809745	-29.537734	5.349878
H	39.929279	-30.110590	7.018337

H	35.294606	-23.539234	11.290421
H	34.473880	-31.378884	3.849386
H	33.996997	-32.930614	4.575678
H	32.862786	-31.562241	4.561696
H	33.840351	-31.797610	6.823858
H	35.484394	-31.685710	6.150085
H	32.727098	-27.079295	8.423753
H	31.839291	-26.425662	7.063016
H	31.502018	-28.077193	7.619841
H	32.181885	-27.024443	1.937851
H	36.886358	-26.569334	9.593267
H	37.622358	-29.595086	4.035274
H	32.330430	-23.016793	6.891397
S	36.103357	-25.012953	4.574792
C	37.417721	-24.513851	5.751743
H	36.996839	-24.050964	6.651531
H	38.029422	-25.368984	6.060047
H	38.070471	-23.782310	5.261185

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B3LYP Scan/Thiolate IPC Model/Trip/40 degrees Constrained Optimization

C	30.490100	-24.755773	2.275807
C	35.662204	-24.529192	10.764576
C	39.150548	-29.963784	6.083324
C	33.537745	-28.810166	0.536741
N	33.122304	-25.545768	4.831436
N	34.625002	-25.474929	7.283948
N	34.746448	-27.679672	3.906194
C	32.774781	-26.794804	2.760911
C	32.881885	-23.886719	6.616528
C	36.352455	-26.618079	8.582671
C	36.811266	-28.912164	4.356874
C	30.637982	-22.732883	4.822438
C	33.393089	-22.632574	9.402603
C	38.758525	-28.529162	8.978521
C	36.331587	-30.131370	1.546678
C	32.457987	-25.785063	3.664469
C	33.830754	-24.385009	7.505371
C	36.795140	-27.487320	7.592045
C	35.725591	-28.565620	3.559934
C	31.410073	-24.795109	3.460280
C	34.079051	-23.838666	8.831428
C	37.942805	-28.371823	7.729067
C	35.458469	-29.129942	2.243489
C	31.473495	-23.943914	4.530080
C	35.030890	-24.638318	9.407701
C	38.107335	-28.974536	6.511493
C	34.284312	-28.572420	1.815953
C	32.544912	-24.437930	5.384787
C	35.366093	-25.649989	8.418351
C	37.039415	-28.473807	5.657249
C	33.865907	-27.650438	2.861911
N	36.269368	-27.574711	6.333963
Fe	34.668682	-26.600148	5.609538
C	34.584317	-31.353898	6.542763
C	34.609730	-31.954461	5.142441
C	32.134839	-27.335147	7.189803
C	33.324376	-27.884448	6.440343
C	33.318883	-29.334092	6.405254
O	32.321846	-30.037046	6.243107
O	34.559443	-29.925341	6.531293
H	29.886457	-22.563707	4.043482
H	31.250868	-21.823532	4.890123
H	30.102403	-22.828289	5.777228
H	31.043327	-24.631055	1.334619
H	29.906644	-25.682286	2.182224
H	29.777383	-23.926988	2.347385
H	33.359443	-27.874188	-0.009830

H	34.091048	-29.478239	-0.132256
H	32.554809	-29.267258	0.717388
H	35.963337	-30.350616	0.538509
H	37.363923	-29.769307	1.447264
H	36.377658	-31.084892	2.091438
H	33.761035	-22.400415	10.408011
H	32.306296	-22.777902	9.476718
H	33.553280	-21.741958	8.779484
H	36.748636	-24.378350	10.696900
H	35.504685	-25.437452	11.362803
H	39.578010	-29.241801	8.835356
H	39.204577	-27.577198	9.299205
H	38.150684	-28.894769	9.818017
H	38.705824	-30.923975	5.787266
H	39.724140	-29.598913	5.220134
H	39.865814	-30.170074	6.887311
H	35.249978	-23.688654	11.333280
H	35.448379	-31.553726	4.569029
H	34.710715	-33.045732	5.196741
H	33.685673	-31.716410	4.613948
H	33.720169	-31.728177	7.098200
H	35.496833	-31.607966	7.089984
H	32.462528	-26.800579	8.090985
H	31.570368	-26.604667	6.600032
H	31.443168	-28.128323	7.491787
H	32.161342	-26.874139	1.868758
H	36.865003	-26.649808	9.539434
H	37.518899	-29.625370	3.944816
H	32.327501	-23.007541	6.930642
S	36.106633	-24.993554	4.550438
C	37.408671	-24.512694	5.748029
H	36.978727	-24.061229	6.649279
H	38.015226	-25.373237	6.051302
H	38.067760	-23.776071	5.273890

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B3LYP Scan/Thiolate IPC Model/Trip/50 degrees Constrained Optimization

C	30.497438	-24.738395	2.270953
C	35.656551	-24.528462	10.767864
C	39.124105	-29.987110	6.103447
C	33.549006	-28.786866	0.528860
N	33.120205	-25.538060	4.833536
N	34.614260	-25.475703	7.289108
N	34.750887	-27.666190	3.903243
C	32.779664	-26.779990	2.757793
C	32.886771	-23.873450	6.614606
C	36.330517	-26.630082	8.593215
C	36.808857	-28.907305	4.360455
C	30.646144	-22.716115	4.818577
C	33.407664	-22.614481	9.396835
C	38.721002	-28.559277	9.000398
C	36.343145	-30.109341	1.540638
C	32.458891	-25.774126	3.664169
C	33.830092	-24.377611	7.506370
C	36.774153	-27.500139	7.603561
C	35.730372	-28.551839	3.557469
C	31.414693	-24.780505	3.457358
C	34.081704	-23.829773	8.830939
C	37.915849	-28.391684	7.745440
C	35.467333	-29.110730	2.237979
C	31.478381	-23.929569	4.526995
C	35.024443	-24.637102	9.411274
C	38.085741	-28.990954	6.526912
C	34.293494	-28.552617	1.809890
C	32.545861	-24.427599	5.384556
C	35.351547	-25.654812	8.425299
C	37.027652	-28.480076	5.666407
C	33.872364	-27.633973	2.857606

N	36.257424	-27.579857	6.341179
Fe	34.667287	-26.593590	5.608925
C	34.509324	-31.386917	6.493352
C	34.652252	-31.939958	5.080958
C	32.196931	-27.375917	7.284451
C	33.321647	-27.888009	6.419505
C	33.295920	-29.337673	6.314385
O	32.311076	-30.011437	6.023183
O	34.509248	-29.956745	6.534719
H	29.909648	-22.532469	4.028621
H	31.264261	-21.812211	4.907417
H	30.093283	-22.818241	5.762929
H	31.054072	-24.627623	1.330079
H	29.902467	-25.658168	2.183000
H	29.795154	-23.900125	2.335060
H	33.411129	-27.856277	-0.038804
H	34.081060	-29.489869	-0.121240
H	32.547912	-29.201502	0.711016
H	35.969335	-30.337759	0.536582
H	37.371796	-29.739495	1.431300
H	36.400886	-31.058634	2.091408
H	33.779681	-22.380154	10.400259
H	32.319637	-22.749192	9.473689
H	33.575037	-21.728859	8.768543
H	36.742848	-24.376349	10.699832
H	35.500423	-25.437366	11.365415
H	39.544641	-29.267046	8.856937
H	39.160197	-27.608958	9.334982
H	38.107351	-28.936156	9.830714
H	38.674241	-30.945287	5.808349
H	39.702138	-29.627706	5.240946
H	39.836067	-30.196078	6.909695
H	35.243705	-23.688865	11.337566
H	35.552213	-31.546812	4.603506
H	34.717842	-33.034990	5.105462
H	33.789600	-31.656534	4.476672
H	33.591523	-31.762096	6.953809
H	35.363316	-31.677562	7.111985
H	31.823901	-26.399872	6.969570
H	31.354546	-28.078447	7.294132
H	32.535867	-27.255557	8.326072
H	32.168797	-26.857106	1.863655
H	36.838970	-26.665249	9.552083
H	37.517289	-29.620087	3.948932
H	32.338659	-22.989159	6.925364
S	36.113103	-24.982978	4.567546
C	37.414766	-24.519792	5.772528
H	36.985450	-24.070228	6.675056
H	38.013522	-25.386860	6.072549
H	38.081259	-23.785523	5.305088

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B3LYP Scan/Thiolate IPC Model/Trip/60 degrees Constrained Optimization

C	30.490285	-24.726643	2.271657
C	35.654880	-24.541447	10.764961
C	39.111258	-29.999483	6.088495
C	33.546042	-28.766318	0.511445
N	33.124846	-25.522611	4.823067
N	34.617724	-25.470992	7.279758
N	34.754850	-27.649753	3.884648
C	32.786254	-26.755747	2.741533
C	32.883615	-23.871522	6.615420
C	36.333360	-26.630787	8.580149
C	36.800542	-28.908893	4.346496
C	30.627019	-22.721738	4.833412
C	33.401274	-22.626164	9.404190
C	38.718753	-28.566393	8.984220
C	36.327291	-30.111148	1.527801

C	32.463123	-25.755777	3.653320
C	33.830588	-24.376151	7.503115
C	36.774261	-27.500668	7.589232
C	35.726678	-28.544511	3.540993
C	31.411524	-24.768247	3.454975
C	34.080430	-23.835004	8.830701
C	37.912538	-28.396557	7.730264
C	35.460209	-29.103053	2.222226
C	31.470223	-23.924752	4.530667
C	35.025261	-24.642916	9.406683
C	38.078045	-28.998156	6.512333
C	34.292006	-28.534823	1.792062
C	32.543368	-24.420633	5.382750
C	35.354665	-25.654799	8.415475
C	37.021391	-28.483070	5.652585
C	33.876521	-27.612918	2.839158
N	36.256048	-27.578233	6.327170
Fe	34.673654	-26.579769	5.593504
C	34.455036	-31.394822	6.567137
C	34.734427	-31.943202	5.173119
C	32.224315	-27.389764	7.299030
C	33.322442	-27.877973	6.387507
C	33.300635	-29.327445	6.248403
O	32.362570	-29.981080	5.806839
O	34.466219	-29.963559	6.625163
H	29.884526	-22.541620	4.048251
H	31.235669	-21.811589	4.924310
H	30.080018	-22.835176	5.779883
H	31.042653	-24.603195	1.329819
H	29.904829	-25.652012	2.178855
H	29.779420	-23.896319	2.344130
H	33.393672	-27.831924	-0.045913
H	34.085416	-29.455124	-0.147799
H	32.551367	-29.196520	0.692947
H	35.952364	-30.338236	0.523850
H	37.359680	-29.751638	1.418642
H	36.375113	-31.059453	2.081028
H	33.775799	-22.393701	10.407115
H	32.314384	-22.767980	9.484856
H	33.560561	-21.736960	8.778914
H	36.742255	-24.396213	10.699633
H	35.491610	-25.450678	11.360197
H	39.543541	-29.272319	8.838208
H	39.156550	-27.616248	9.321001
H	38.106389	-28.946544	9.814021
H	38.657196	-30.957963	5.800673
H	39.685836	-29.646240	5.221204
H	39.826814	-30.206455	6.892095
H	35.246224	-23.700464	11.335646
H	35.680376	-31.555556	4.788947
H	34.791447	-33.038664	5.201450
H	33.938159	-31.652709	4.487216
H	33.491233	-31.763186	6.929424
H	35.238053	-31.699962	7.267208
H	31.861410	-26.395261	7.033432
H	31.366854	-28.075927	7.290107
H	32.578499	-27.322370	8.340866
H	32.174619	-26.829953	1.847667
H	36.841864	-26.669034	9.538869
H	37.504383	-29.626604	3.935730
H	32.331339	-22.991947	6.932160
S	36.122967	-24.971232	4.562036
C	37.423807	-24.516106	5.771117
H	36.993612	-24.069932	6.674883
H	38.020267	-25.385779	6.068103
H	38.092544	-23.780972	5.308265

B3LYP Scan/Thiolate IPC Model/Trip/70 degrees Constrained Optimization

C	30.508188	-24.563280	2.265761
C	35.672219	-24.682384	10.761921
C	39.094520	-30.016257	5.910400
C	33.453805	-28.652390	0.428111
N	33.125011	-25.471625	4.798871
N	34.626079	-25.495118	7.249577
N	34.719559	-27.596842	3.800417
C	32.771937	-26.636872	2.679239
C	32.880825	-23.884300	6.648904
C	36.361893	-26.681002	8.499624
C	36.719471	-28.937168	4.241728
C	30.643642	-22.657470	4.901372
C	33.387126	-22.746869	9.485975
C	38.764315	-28.607784	8.827754
C	36.174663	-30.120332	1.432203
C	32.464963	-25.658115	3.618547
C	33.829008	-24.418942	7.518181
C	36.786398	-27.535381	7.487670
C	35.652710	-28.529362	3.448356
C	31.423047	-24.655527	3.451073
C	34.079769	-23.923587	8.864095
C	37.925122	-28.434314	7.596070
C	35.358412	-29.072122	2.128605
C	31.481985	-23.852997	4.557819
C	35.039166	-24.738855	9.402828
C	38.059058	-29.032955	6.371546
C	34.215674	-28.453118	1.704396
C	32.547642	-24.385825	5.394941
C	35.373004	-25.711237	8.373590
C	36.980963	-28.513723	5.541950
C	33.839352	-27.523676	2.759987
N	36.241062	-27.601877	6.236629
Fe	34.668408	-26.556251	5.529572
C	34.261748	-31.381209	7.089327
C	35.383800	-31.915663	6.210714
C	31.979808	-27.490119	6.800101
C	33.351974	-27.888883	6.319198
C	33.452051	-29.337256	6.132357
O	32.908821	-30.004244	5.269369
O	34.219988	-29.948078	7.109087
H	29.899259	-22.450649	4.124673
H	31.254958	-21.752147	5.019001
H	30.099218	-22.799348	5.845471
H	31.064961	-24.395555	1.333344
H	29.926458	-25.485364	2.127874
H	29.793985	-23.739481	2.372052
H	33.294995	-27.704530	-0.103859
H	33.984821	-29.324578	-0.254709
H	32.461440	-29.087462	0.611625
H	35.798819	-30.315371	0.421812
H	37.227453	-29.820662	1.338390
H	36.160855	-31.075490	1.975824
H	33.764017	-22.546515	10.494945
H	32.302732	-22.906958	9.566821
H	33.530035	-21.832377	8.893893
H	36.759862	-24.538714	10.698358
H	35.507527	-25.609904	11.327893
H	39.576238	-29.324428	8.662939
H	39.222382	-27.661336	9.147504
H	38.170066	-28.976517	9.675459
H	38.647365	-30.973594	5.609029
H	39.650240	-29.636836	5.041923
H	39.825240	-30.231654	6.697956
H	35.267739	-23.858669	11.360250
H	36.345314	-31.504590	6.526681
H	35.430828	-33.009964	6.273379
H	35.215124	-31.632342	5.170765

H	33.296349	-31.764802	6.750495
H	34.414350	-31.670185	8.133702
H	31.930062	-26.440407	7.088172
H	31.212265	-27.653475	6.024354
H	31.665809	-28.086090	7.673568
H	32.158033	-26.677459	1.784727
H	36.884572	-26.737515	9.449719
H	37.389893	-29.681024	3.822124
H	32.325609	-23.018787	6.997547
S	36.139605	-24.962472	4.516585
C	37.413304	-24.496102	5.749939
H	36.962587	-24.058351	6.647575
H	38.014201	-25.360237	6.054471
H	38.081733	-23.752328	5.300577

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B3LYP Scan/Thiolate IPC Model/Trip/80 degrees Constrained Optimization

C	30.523519	-24.505075	2.238463
C	35.663405	-24.734098	10.749319
C	39.060892	-30.050955	5.854427
C	33.449939	-28.592423	0.370566
N	33.114720	-25.465195	4.779065
N	34.617648	-25.511695	7.228725
N	34.710679	-27.579083	3.757869
C	32.772291	-26.597091	2.639689
C	32.865019	-23.901464	6.648780
C	36.359780	-26.704063	8.463880
C	36.698908	-28.938780	4.192301
C	30.643317	-22.642903	4.905524
C	33.367620	-22.795301	9.497728
C	38.757702	-28.638873	8.775070
C	36.150949	-30.095947	1.373483
C	32.462718	-25.630837	3.591034
C	33.815168	-24.443167	7.511169
C	36.781447	-27.551467	7.444981
C	35.636723	-28.516292	3.400813
C	31.426031	-24.621972	3.431013
C	34.065242	-23.961726	8.862158
C	37.915638	-28.456892	7.546445
C	35.342701	-29.045330	2.075300
C	31.478477	-23.837529	4.551040
C	35.029931	-24.777718	9.390014
C	38.041107	-29.053820	6.319976
C	34.207679	-28.412457	1.652111
C	32.536088	-24.386561	5.387414
C	35.367252	-25.736640	8.349264
C	36.964745	-28.524673	5.494820
C	33.834641	-27.490098	2.715335
N	36.232054	-27.610851	6.195136
Fe	34.660153	-26.555664	5.496627
C	34.243518	-31.350272	7.266843
C	35.486921	-31.860834	6.552806
C	31.989481	-27.542221	6.785893
C	33.363771	-27.904890	6.287759
C	33.526949	-29.353637	6.143275
O	33.142310	-30.056947	5.227425
O	34.152216	-29.919471	7.243738
H	29.905261	-22.421895	4.126700
H	31.258206	-21.742267	5.039488
H	30.091917	-22.794846	5.843991
H	31.090723	-24.324236	1.314828
H	29.938482	-25.421538	2.078710
H	29.812563	-23.679410	2.351780
H	33.301208	-27.637724	-0.152058
H	33.978690	-29.261612	-0.316923
H	32.453133	-29.021420	0.544426
H	35.784086	-30.270947	0.356114
H	37.209223	-29.811564	1.296042

H	36.115412	-31.058260	1.903320
H	33.743968	-22.604538	10.508753
H	32.283953	-22.960900	9.577027
H	33.506372	-21.873507	8.916011
H	36.750793	-24.588162	10.686942
H	35.500208	-25.667633	11.305766
H	39.563317	-29.361694	8.606355
H	39.224262	-27.696420	9.094290
H	38.163615	-29.003909	9.624430
H	38.596932	-31.003152	5.562122
H	39.614024	-29.682894	4.979544
H	39.795238	-30.272396	6.636921
H	35.257807	-23.917145	11.356131
H	36.384697	-31.403207	6.974488
H	35.565427	-32.950570	6.652522
H	35.441333	-31.608954	5.492411
H	33.342620	-31.776961	6.818345
H	34.271093	-31.610593	8.329456
H	31.907407	-26.486896	7.046525
H	31.211885	-27.751897	6.030408
H	31.714005	-28.125645	7.680802
H	32.163745	-26.622764	1.740936
H	36.884592	-26.767816	9.412309
H	37.362976	-29.685754	3.768227
H	32.307466	-23.041647	7.007648
S	36.131841	-24.954133	4.497068
C	37.398802	-24.490660	5.738368
H	36.942926	-24.060461	6.637038
H	38.001582	-25.354632	6.039779
H	38.066348	-23.741707	5.296395

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B3LYP Scan/Thiolate IPC Model/Trip/90 degrees Constrained Optimization

C	30.499650	-24.550064	2.251150
C	35.688156	-24.695232	10.735296
C	39.048788	-30.074295	5.884497
C	33.511183	-28.558017	0.348593
N	33.115561	-25.471585	4.780799
N	34.625303	-25.500512	7.226026
N	34.743356	-27.556506	3.749791
C	32.793497	-26.595586	2.634042
C	32.852047	-23.911041	6.651301
C	36.372771	-26.683925	8.463509
C	36.731552	-28.914527	4.191526
C	30.593122	-22.695730	4.924325
C	33.373415	-22.777250	9.486280
C	38.745192	-28.647618	8.796911
C	36.220619	-30.042122	1.355489
C	32.464234	-25.643689	3.593131
C	33.816884	-24.435807	7.507669
C	36.792803	-27.537905	7.449640
C	35.678668	-28.484040	3.392274
C	31.408021	-24.654355	3.440507
C	34.073025	-23.944212	8.853762
C	37.916303	-28.455613	7.560884
C	35.398761	-29.004155	2.060265
C	31.449366	-23.873311	4.563483
C	35.045665	-24.751580	9.380623
C	38.044070	-29.056122	6.336514
C	34.260153	-28.379409	1.635423
C	32.520194	-24.405058	5.394194
C	35.381250	-25.715641	8.344180
C	36.982953	-28.512808	5.500821
C	33.871120	-27.470273	2.704214
N	36.251456	-27.593990	6.195708
Fe	34.674886	-26.544172	5.491771
C	34.069129	-31.418697	7.167458
C	35.386931	-31.914692	6.587271

C	32.060611	-27.542633	6.869986
C	33.397926	-27.907362	6.282826
C	33.538410	-29.348171	6.068201
O	33.251409	-29.995542	5.079310
O	34.003492	-29.987730	7.211352
H	29.846660	-22.488191	4.149784
H	31.191019	-21.783324	5.055867
H	30.049892	-22.859167	5.865604
H	31.059528	-24.348264	1.327310
H	29.936586	-25.479158	2.085683
H	29.769125	-23.742823	2.372610
H	33.343883	-27.599926	-0.161884
H	34.056583	-29.206697	-0.345609
H	32.523261	-29.010802	0.512960
H	35.874183	-30.198021	0.327881
H	37.280144	-29.756875	1.304573
H	36.174130	-31.014215	1.866453
H	33.757899	-22.575811	10.492168
H	32.291601	-22.949190	9.577143
H	33.500714	-21.859502	8.895690
H	36.774425	-24.545164	10.664337
H	35.532810	-25.625252	11.299881
H	39.551900	-29.369912	8.631181
H	39.209401	-27.707972	9.127596
H	38.142360	-29.018176	9.637744
H	38.570634	-31.025175	5.610986
H	39.603751	-29.729807	5.001254
H	39.783149	-30.291919	6.668080
H	35.283088	-23.875580	11.338813
H	36.232366	-31.499335	7.141685
H	35.439772	-33.009460	6.634642
H	35.477746	-31.605571	5.545073
H	33.227493	-31.802760	6.585336
H	33.958367	-31.736900	8.208791
H	32.041048	-26.523077	7.257678
H	31.252218	-27.616473	6.121395
H	31.782134	-28.217082	7.696099
H	32.186842	-26.624817	1.734124
H	36.896256	-26.744640	9.412897
H	37.398169	-29.660153	3.769062
H	32.285546	-23.057677	7.011560
S	36.135401	-24.923513	4.499981
C	37.402659	-24.461878	5.741681
H	36.947091	-24.035219	6.642221
H	38.006684	-25.326174	6.039625
H	38.069032	-23.710655	5.301758

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B3LYP Scan/Thiolate IPC Model/Trip/100 degrees Constrained Optimization

C	30.494976	-24.558134	2.245354
C	35.682951	-24.704610	10.730062
C	39.047212	-30.079762	5.877005
C	33.551025	-28.518364	0.315913
N	33.113928	-25.475150	4.773460
N	34.624712	-25.504009	7.218150
N	34.760991	-27.539263	3.731520
C	32.806820	-26.585342	2.617468
C	32.841682	-23.922888	6.649493
C	36.372463	-26.687760	8.455270
C	36.750375	-28.895491	4.173124
C	30.570836	-22.719050	4.929424
C	33.362882	-22.790572	9.484701
C	38.736519	-28.661308	8.792328
C	36.263986	-29.995692	1.323518
C	32.465952	-25.644783	3.583552
C	33.811924	-24.443014	7.502454
C	36.795099	-27.538694	7.439953
C	35.702452	-28.459068	3.371073

C	31.402017	-24.663114	3.435712
C	34.066440	-23.953731	8.849562
C	37.914882	-28.460676	7.552825
C	35.432386	-28.968951	2.033153
C	31.436084	-23.888346	4.563300
C	35.041448	-24.759367	9.374866
C	38.046462	-29.056792	6.326721
C	34.292090	-28.347574	1.608366
C	32.510529	-24.416228	5.391935
C	35.380434	-25.719830	8.336420
C	36.992522	-28.505247	5.487435
C	33.892363	-27.450522	2.683455
N	36.259042	-27.588314	6.183231
Fe	34.679848	-26.541217	5.480128
C	33.967652	-31.437099	7.177520
C	35.321669	-31.928903	6.681635
C	32.114179	-27.556356	6.932307
C	33.415540	-27.914714	6.266416
C	33.567246	-29.351257	6.052084
O	33.387336	-29.990795	5.033027
O	33.900314	-30.007649	7.235534
H	29.822520	-22.514098	4.155972
H	31.161644	-21.802524	5.064422
H	30.029297	-22.890505	5.870244
H	31.054038	-24.338315	1.325078
H	29.945186	-25.492952	2.068146
H	29.753123	-23.762396	2.373925
H	33.384512	-27.556925	-0.188554
H	34.101995	-29.160690	-0.379806
H	32.563171	-28.974623	0.470921
H	35.924684	-30.143646	0.292357
H	37.322225	-29.704297	1.281878
H	36.219429	-30.972660	1.825200
H	33.745209	-22.591355	10.491840
H	32.281378	-22.965579	9.573264
H	33.488772	-21.870654	8.897206
H	36.768318	-24.547569	10.660294
H	35.533020	-25.637955	11.290575
H	39.545387	-29.380944	8.625677
H	39.197149	-27.723509	9.133028
H	38.129447	-29.039369	9.626769
H	38.565049	-31.029190	5.605572
H	39.603721	-29.739616	4.993087
H	39.780489	-30.298759	6.661193
H	35.272532	-23.890031	11.336801
H	36.129587	-31.508612	7.286326
H	35.377008	-33.023301	6.734100
H	35.473894	-31.620606	5.646599
H	33.168193	-31.813534	6.533510
H	33.784401	-31.768751	8.204329
H	32.113256	-26.541567	7.332589
H	31.268244	-27.621028	6.225439
H	31.882053	-28.243535	7.760850
H	32.203256	-26.612437	1.715391
H	36.893087	-26.751666	9.406004
H	37.419418	-29.638036	3.749122
H	32.270518	-23.073955	7.012809
S	36.133298	-24.905297	4.499727
C	37.399423	-24.449308	5.744656
H	36.942733	-24.030484	6.648293
H	38.005709	-25.314225	6.036148
H	38.063843	-23.693145	5.310280

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B3LYP Scan/Thiolate IPC Model/Trip/110 degrees Constrained Optimization

C	30.522128	-24.531372	2.199865
C	35.617143	-24.747334	10.738414
C	39.041606	-30.074743	5.873544

C	33.576864	-28.498831	0.285777
N	33.120120	-25.462066	4.744178
N	34.603737	-25.514187	7.206230
N	34.767933	-27.530318	3.710858
C	32.827637	-26.563873	2.582594
C	32.828710	-23.925875	6.630182
C	36.336709	-26.708967	8.454346
C	36.750366	-28.892270	4.163068
C	30.573495	-22.708496	4.895944
C	33.311571	-22.823468	9.482090
C	38.706376	-28.675227	8.795358
C	36.277946	-29.988666	1.309520
C	32.482274	-25.624885	3.548394
C	33.787657	-24.455211	7.489716
C	36.770577	-27.550875	7.436431
C	35.707981	-28.453051	3.355228
C	31.420053	-24.641701	3.396588
C	34.024173	-23.979545	8.844258
C	37.892028	-28.470418	7.551767
C	35.444857	-28.960250	2.014914
C	31.443494	-23.873990	4.529078
C	34.992554	-24.789992	9.374925
C	38.033671	-29.058796	6.323164
C	34.310218	-28.333203	1.583259
C	32.510937	-24.407442	5.364165
C	35.345606	-25.740107	8.332137
C	36.983826	-28.505425	5.479833
C	33.907175	-27.435626	2.656718
N	36.243733	-27.593207	6.175347
Fe	34.675193	-26.537470	5.463924
C	33.964680	-31.416602	7.171806
C	35.304022	-31.927363	6.655428
C	32.248043	-27.541451	7.133363
C	33.393034	-27.907067	6.225287
C	33.554479	-29.340993	6.025904
O	33.344744	-29.994267	5.020795
O	33.909247	-29.986365	7.211852
H	29.829551	-22.501104	4.118911
H	31.161361	-21.791371	5.039723
H	30.026424	-22.886240	5.832391
H	31.088307	-24.308502	1.284704
H	29.973148	-25.465207	2.015095
H	29.779878	-23.735603	2.325925
H	33.441322	-27.539309	-0.231798
H	34.116249	-29.164320	-0.397044
H	32.575555	-28.925768	0.437147
H	35.929553	-30.152447	0.283850
H	37.333380	-29.689009	1.253525
H	36.246826	-30.959312	1.824064
H	33.676641	-22.637739	10.498158
H	32.228582	-22.998298	9.549721
H	33.448589	-21.896183	8.908865
H	36.701228	-24.575346	10.684282
H	35.472625	-25.690801	11.283037
H	39.517082	-29.393216	8.630554
H	39.163874	-27.738324	9.142682
H	38.094741	-29.057521	9.624519
H	38.565074	-31.023142	5.589032
H	39.605119	-29.724720	4.997931
H	39.768320	-30.298613	6.662440
H	35.189125	-23.947248	11.352181
H	36.127731	-31.509706	7.240338
H	35.348972	-33.021909	6.717562
H	35.439622	-31.631375	5.614453
H	33.149254	-31.794911	6.549371
H	33.799641	-31.733842	8.206348
H	31.868761	-26.541303	6.918870
H	31.403680	-28.242284	7.044682

H	32.546695	-27.544183	8.195243
H	32.231692	-26.586470	1.675340
H	36.847443	-26.780042	9.409903
H	37.421993	-29.633826	3.741407
H	32.253795	-23.080137	6.995031
S	36.138396	-24.899679	4.511700
C	37.404357	-24.472521	5.766684
H	36.947389	-24.066618	6.676079
H	38.005194	-25.345564	6.044736
H	38.073723	-23.712574	5.346825

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B3LYP Scan/Thiolate IPC Model/Trip/120 degrees Constrained Optimization

C	30.501537	-24.557656	2.218677
C	35.648032	-24.732388	10.728250
C	39.065243	-30.059582	5.858101
C	33.601698	-28.476223	0.274654
N	33.121176	-25.467990	4.748373
N	34.614178	-25.513280	7.204867
N	34.796129	-27.503740	3.697058
C	32.837287	-26.560433	2.581346
C	32.820278	-23.941765	6.641212
C	36.362593	-26.695603	8.443639
C	36.784527	-28.859357	4.143321
C	30.542745	-22.745498	4.921938
C	33.316119	-22.830726	9.487175
C	38.730746	-28.664461	8.781284
C	36.319484	-29.944210	1.287154
C	32.481151	-25.632429	3.553763
C	33.790386	-24.461616	7.493685
C	36.797292	-27.534868	7.423692
C	35.742694	-28.417451	3.336832
C	31.405973	-24.662405	3.411065
C	34.032643	-23.982562	8.845937
C	37.918175	-28.455315	7.537258
C	35.481008	-28.922508	1.995531
C	31.424787	-23.899309	4.546942
C	35.012152	-24.783872	9.370228
C	38.059945	-29.041020	6.307484
C	34.339078	-28.305799	1.569203
C	32.501976	-24.423098	5.375296
C	35.365488	-25.732245	8.325946
C	37.012203	-28.483825	5.464179
C	33.930430	-27.415769	2.646808
N	36.270789	-27.574564	6.162242
Fe	34.690261	-26.530611	5.456901
C	33.767276	-31.476760	7.091641
C	35.176511	-31.990129	6.820403
C	32.303703	-27.562254	7.141035
C	33.434774	-27.924118	6.213678
C	33.588775	-29.348563	5.977145
O	33.528983	-29.962496	4.926833
O	33.726743	-30.050557	7.182337
H	29.793020	-22.544010	4.148923
H	31.120452	-21.822031	5.066332
H	30.001919	-22.932718	5.860174
H	31.060039	-24.318046	1.303017
H	29.967405	-25.498984	2.028604
H	29.746593	-23.775450	2.354017
H	33.457247	-27.517698	-0.242460
H	34.142840	-29.138027	-0.410338
H	32.604029	-28.910155	0.430186
H	35.966661	-30.113408	0.263875
H	37.371993	-29.635599	1.224694
H	36.299078	-30.913506	1.804680
H	33.686142	-22.641532	10.500811
H	32.234724	-23.012542	9.561619
H	33.443530	-21.903125	8.912245

H	36.729310	-24.546591	10.664439
H	35.520385	-25.677166	11.274777
H	39.538023	-29.386355	8.616910
H	39.192748	-27.729875	9.129066
H	38.116880	-29.043739	9.610191
H	38.586486	-31.006947	5.573810
H	39.629860	-29.711450	4.982458
H	39.791174	-30.285113	6.647187
H	35.215203	-23.937386	11.345236
H	35.876224	-31.608784	7.569154
H	35.201440	-33.086597	6.844994
H	35.512283	-31.656636	5.837230
H	33.083764	-31.812751	6.307312
H	33.401619	-31.834134	8.059852
H	31.879615	-26.588707	6.888762
H	31.489136	-28.300420	7.122107
H	32.639072	-27.494436	8.188794
H	32.238022	-26.587639	1.676401
H	36.876939	-26.764689	9.397420
H	37.458298	-29.596848	3.718012
H	32.238504	-23.102866	7.010941
S	36.135257	-24.869602	4.510320
C	37.398706	-24.433341	5.764643
H	36.939370	-24.033951	6.675753
H	38.008304	-25.301250	6.039878
H	38.060224	-23.666121	5.345578

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B3LYP_Scan/Thiolate_IPC_Model/Trip/130 degrees Constrained Optimization

C	30.507852	-24.528022	2.206187
C	35.622326	-24.844215	10.729804
C	39.115924	-30.018372	5.746294
C	33.623116	-28.404442	0.202769
N	33.121145	-25.477465	4.727838
N	34.614406	-25.553890	7.184357
N	34.801876	-27.491528	3.647499
C	32.837637	-26.541592	2.546461
C	32.818688	-23.977188	6.641295
C	36.366039	-26.749771	8.404835
C	36.811904	-28.823821	4.062395
C	30.550998	-22.749448	4.931586
C	33.291078	-22.925614	9.513837
C	38.763973	-28.690818	8.699247
C	36.357825	-29.860226	1.187319
C	32.481825	-25.625845	3.530602
C	33.784951	-24.511719	7.489279
C	36.811113	-27.563385	7.368162
C	35.760590	-28.384526	3.268317
C	31.409329	-24.651449	3.399043
C	34.017233	-24.060077	8.852893
C	37.945813	-28.468813	7.461174
C	35.504413	-28.866672	1.917614
C	31.429546	-23.901784	4.543988
C	34.996744	-24.868279	9.366390
C	38.094159	-29.027168	6.219347
C	34.354161	-28.256656	1.503760
C	32.504235	-24.438393	5.367039
C	35.361397	-25.792425	8.304342
C	37.036167	-28.470589	5.389189
C	33.935583	-27.392211	2.598698
N	36.282192	-27.587043	6.107100
Fe	34.692028	-26.547216	5.423680
C	33.651215	-31.444374	7.277496
C	35.094813	-31.929445	7.343714
C	32.265165	-27.567719	7.045533
C	33.445249	-27.943405	6.186568
C	33.666211	-29.369168	6.051359
O	33.836443	-30.031369	5.042045

O	33.566788	-30.019069	7.294188
H	29.801771	-22.537546	4.160912
H	31.131555	-21.829343	5.085603
H	30.009942	-22.945135	5.867943
H	31.067483	-24.265157	1.297537
H	29.980939	-25.468752	1.994539
H	29.747008	-23.754113	2.355518
H	33.487502	-27.437574	-0.301284
H	34.164788	-29.059143	-0.488584
H	32.621736	-28.834504	0.344908
H	36.003529	-30.017521	0.162617
H	37.404166	-29.531097	1.125782
H	36.357571	-30.838467	1.687874
H	33.648925	-22.760322	10.535974
H	32.209408	-23.111567	9.571354
H	33.422729	-21.983914	8.963239
H	36.703403	-24.653467	10.678134
H	35.493842	-25.801176	11.254521
H	39.576883	-29.403010	8.520934
H	39.218997	-27.758061	9.060834
H	38.155809	-29.088729	9.523621
H	38.650949	-30.960466	5.424556
H	39.684509	-29.633666	4.888619
H	39.836611	-30.262438	6.534526
H	35.182283	-24.064298	11.360765
H	35.603480	-31.508234	8.215408
H	35.134215	-33.023637	7.413317
H	35.634839	-31.617614	6.448434
H	33.163032	-31.829567	6.378375
H	33.089398	-31.775100	8.157343
H	31.835351	-26.613860	6.737298
H	31.469996	-28.325344	7.022333
H	32.553333	-27.454799	8.102904
H	32.238945	-26.556946	1.640815
H	36.879793	-26.833395	9.357742
H	37.494595	-29.544158	3.622372
H	32.235271	-23.144807	7.022904
S	36.127565	-24.864375	4.493479
C	37.383932	-24.429725	5.755483
H	36.918724	-24.048054	6.671132
H	38.003760	-25.293856	6.020042
H	38.036772	-23.649134	5.347649

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B3LYP Scan/Thiolate IPC Model/Trip/140 degrees Constrained Optimization

C	30.491059	-24.547224	2.218107
C	35.629276	-24.877074	10.725421
C	39.148260	-29.991941	5.699248
C	33.634450	-28.384713	0.180240
N	33.121379	-25.489648	4.724263
N	34.619845	-25.571623	7.177617
N	34.813114	-27.483590	3.628169
C	32.832840	-26.550024	2.541777
C	32.823791	-23.992878	6.641442
C	36.372562	-26.772570	8.390759
C	36.843455	-28.789698	4.024105
C	30.546034	-22.767946	4.943061
C	33.300681	-22.950496	9.517080
C	38.777106	-28.707919	8.669461
C	36.398406	-29.802205	1.139782
C	32.476258	-25.639118	3.530360
C	33.791529	-24.529732	7.486477
C	36.822163	-27.574556	7.346834
C	35.784881	-28.356868	3.236971
C	31.399823	-24.668184	3.405668
C	34.024896	-24.083623	8.851702
C	37.962147	-28.474097	7.431525
C	35.530851	-28.830678	1.883007

C	31.425005	-23.918258	4.550445
C	35.003181	-24.895422	9.362139
C	38.118392	-29.014134	6.182515
C	34.368062	-28.237114	1.479837
C	32.505400	-24.452367	5.367536
C	35.367010	-25.815367	8.296270
C	37.059411	-28.453791	5.356355
C	33.941031	-27.388101	2.583778
N	36.295997	-27.586854	6.084115
Fe	34.697953	-26.556710	5.412502
C	33.548336	-31.458933	7.284247
C	34.982977	-31.884528	7.577421
C	32.270381	-27.570986	7.020144
C	33.458321	-27.956857	6.176814
C	33.699266	-29.379836	6.074775
O	34.044460	-30.039035	5.107477
O	33.403896	-30.039515	7.284410
H	29.793127	-22.556611	4.175853
H	31.125725	-21.847033	5.095420
H	30.009433	-22.965487	5.881583
H	31.044472	-24.281981	1.306340
H	29.966201	-25.489682	2.009019
H	29.728345	-23.776102	2.372238
H	33.491928	-27.417019	-0.320430
H	34.178221	-29.034017	-0.514552
H	32.635873	-28.820971	0.323224
H	36.037149	-29.963412	0.118115
H	37.436484	-29.449515	1.069016
H	36.425176	-30.781952	1.636541
H	33.659118	-22.789451	10.539689
H	32.218752	-23.135012	9.574335
H	33.433581	-22.007004	8.969870
H	36.710479	-24.686947	10.674036
H	35.500308	-25.835872	11.246673
H	39.592995	-29.415266	8.485576
H	39.227896	-27.777994	9.043519
H	38.167442	-29.117463	9.486991
H	38.689467	-30.930083	5.357946
H	39.720629	-29.589500	4.852246
H	39.864845	-30.246253	6.487961
H	35.190109	-24.099199	11.359517
H	35.329698	-31.446540	8.517894
H	35.057616	-32.976286	7.655167
H	35.643762	-31.546554	6.777668
H	33.224273	-31.861168	6.320823
H	32.869748	-31.816365	8.065897
H	31.851541	-26.614074	6.708466
H	31.472804	-28.324564	6.990348
H	32.549749	-27.461661	8.079906
H	32.229495	-26.567356	1.639249
H	36.885866	-26.862602	9.343335
H	37.535190	-29.496126	3.575801
H	32.240997	-23.161583	7.026338
S	36.119554	-24.854293	4.489660
C	37.374727	-24.419621	5.753037
H	36.908279	-24.046755	6.671687
H	38.000419	-25.281489	6.011206
H	38.022128	-23.632208	5.349651

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B3LYP_Scan/Thiolate_IPC_Model/Trip/150 degrees Constrained Optimization

C	30.467138	-24.583435	2.240259
C	35.641419	-24.897022	10.723040
C	39.196797	-29.945347	5.653610
C	33.636612	-28.386692	0.175523
N	33.125836	-25.500374	4.725480
N	34.636169	-25.576147	7.171494
N	34.829297	-27.474471	3.615928

C	32.825495	-26.569353	2.548689
C	32.834283	-24.001636	6.642052
C	36.392186	-26.778505	8.377315
C	36.889548	-28.738982	3.987887
C	30.540494	-22.789206	4.955030
C	33.311685	-22.967659	9.521352
C	38.802586	-28.709586	8.641742
C	36.440808	-29.746461	1.101841
C	32.470649	-25.658458	3.538241
C	33.805337	-24.537449	7.484238
C	36.848437	-27.566936	7.325850
C	35.816780	-28.323591	3.211182
C	31.387906	-24.693911	3.419599
C	34.037917	-24.096769	8.851354
C	37.993538	-28.460888	7.402845
C	35.559922	-28.796682	1.857556
C	31.420727	-23.937839	4.560312
C	35.016839	-24.909772	9.359022
C	38.160138	-28.979527	6.146114
C	34.379804	-28.227777	1.468428
C	32.510441	-24.463436	5.370299
C	35.383504	-25.823676	8.289033
C	37.100269	-28.415590	5.323687
C	33.946310	-27.391183	2.579458
N	36.327024	-27.566322	6.061050
Fe	34.714923	-26.555886	5.404605
C	33.427213	-31.485272	7.234794
C	34.779581	-31.907346	7.799280
C	32.288409	-27.575684	6.994727
C	33.495188	-27.963440	6.179933
C	33.760952	-29.381564	6.106651
O	34.287074	-30.022450	5.209299
O	33.269198	-30.068427	7.238440
H	29.781672	-22.583111	4.192252
H	31.118237	-21.865916	5.100087
H	30.010982	-22.985115	5.897915
H	31.010844	-24.323481	1.321172
H	29.942393	-25.528545	2.042990
H	29.704091	-23.813040	2.396372
H	33.470877	-27.420883	-0.321615
H	34.186082	-29.024082	-0.525825
H	32.647804	-28.842164	0.326590
H	36.070028	-29.915764	0.084875
H	37.468968	-29.368545	1.017829
H	36.498223	-30.725528	1.597317
H	33.669934	-22.809963	10.544551
H	32.230085	-23.154337	9.577990
H	33.442806	-22.021768	8.977868
H	36.722296	-24.704439	10.673967
H	35.513795	-25.858724	11.239314
H	39.621492	-29.412063	8.452530
H	39.248803	-27.783769	9.031267
H	38.189507	-29.132079	9.450055
H	38.742640	-30.879840	5.296728
H	39.771241	-29.528201	4.815143
H	39.910906	-30.208013	6.441846
H	35.199908	-24.123338	11.360640
H	34.921486	-31.498917	8.804338
H	34.854874	-33.000332	7.855871
H	35.583618	-31.537238	7.160999
H	33.308744	-31.864092	6.216523
H	32.611024	-31.869434	7.856095
H	31.887212	-26.610328	6.688999
H	31.487132	-28.322401	6.934299
H	32.542513	-27.487579	8.062759
H	32.213649	-26.594798	1.652067
H	36.904060	-26.875342	9.330020
H	37.591941	-29.429337	3.531212

H	32.250233	-23.172466	7.029667
S	36.110113	-24.830801	4.478397
C	37.372132	-24.396199	5.735177
H	36.910109	-24.033973	6.660321
H	38.005861	-25.255670	5.981634
H	38.010741	-23.600916	5.333240

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B3LYP Scan/Thiolate IPC Model/Trip/160 degrees Constrained Optimization

C	30.451497	-24.620997	2.260193
C	35.661299	-24.900065	10.721311
C	39.248012	-29.896685	5.623734
C	33.648417	-28.389180	0.175217
N	33.128028	-25.518521	4.733027
N	34.650378	-25.582560	7.172432
N	34.838032	-27.483398	3.618571
C	32.820871	-26.595592	2.561274
C	32.843152	-24.013103	6.645473
C	36.416027	-26.776241	8.371840
C	36.924313	-28.709260	3.971964
C	30.537133	-22.813189	4.965602
C	33.324508	-22.976597	9.524022
C	38.847144	-28.683926	8.620688
C	36.479772	-29.706478	1.080536
C	32.466294	-25.684062	3.550593
C	33.817746	-24.545412	7.485981
C	36.876595	-27.556085	7.315898
C	35.838631	-28.312402	3.203833
C	31.379773	-24.723431	3.434367
C	34.052258	-24.103764	8.852445
C	38.032737	-28.436785	7.385009
C	35.583736	-28.780627	1.848225
C	31.417970	-23.961381	4.570999
C	35.034063	-24.914418	9.358541
C	38.203134	-28.944431	6.124575
C	34.392051	-28.229447	1.467846
C	32.514050	-24.480004	5.376786
C	35.401460	-25.827090	8.287957
C	37.134222	-28.389118	5.308305
C	33.949855	-27.406563	2.585614
N	36.352278	-27.554423	6.052525
Fe	34.726257	-26.565080	5.407701
C	33.301125	-31.513310	7.166054
C	34.569116	-31.926196	7.906359
C	32.301675	-27.576100	6.991777
C	33.515918	-27.972251	6.192584
C	33.787942	-29.388950	6.141984
O	34.465262	-30.016617	5.340076
O	33.119339	-30.099980	7.165633
H	29.774193	-22.611627	4.205757
H	31.113577	-21.888157	5.104392
H	30.012609	-23.006687	5.911760
H	30.989013	-24.364955	1.336380
H	29.927248	-25.568054	2.071145
H	29.688009	-23.851167	2.416863
H	33.474215	-27.422646	-0.317624
H	34.202356	-29.018931	-0.529512
H	32.663498	-28.853334	0.325153
H	36.103622	-29.880791	0.066392
H	37.497600	-29.303314	0.988405
H	36.565982	-30.685676	1.571483
H	33.683823	-22.818763	10.546816
H	32.243416	-23.165711	9.582042
H	33.452809	-22.030072	8.980993
H	36.740987	-24.701298	10.670537
H	35.540151	-25.863285	11.236312
H	39.670337	-29.380053	8.426564
H	39.288249	-27.756463	9.012221

H	38.239397	-29.113412	9.429302
H	38.800927	-30.833117	5.263106
H	39.815769	-29.469219	4.785872
H	39.967122	-30.156823	6.408251
H	35.216660	-24.129954	11.361022
H	34.563400	-31.533689	8.927767
H	34.653278	-33.018836	7.955714
H	35.447084	-31.534145	7.390371
H	33.330746	-31.879516	6.136663
H	32.412935	-31.917843	7.663143
H	31.928479	-26.593811	6.709276
H	31.486204	-28.302389	6.893155
H	32.536765	-27.528875	8.066699
H	32.205264	-26.625637	1.667368
H	36.931389	-26.871900	9.322782
H	37.637315	-29.384081	3.508553
H	32.258817	-23.184207	7.033233
S	36.097111	-24.822732	4.471487
C	37.367592	-24.381215	5.717507
H	36.911068	-24.026700	6.648357
H	38.011284	-25.235896	5.954671
H	37.995121	-23.578576	5.312787

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B3LYP Scan/Thiolate IPC Model/Trip/170 degrees Constrained Optimization

C	30.421179	-24.686167	2.297459
C	35.699108	-24.846590	10.717413
C	39.290059	-29.853017	5.638147
C	33.644441	-28.438091	0.216502
N	33.132674	-25.529540	4.750937
N	34.668098	-25.566166	7.181633
N	34.855365	-27.482960	3.638655
C	32.815879	-26.631946	2.593656
C	32.853618	-24.006482	6.650290
C	36.441250	-26.746496	8.382856
C	36.960163	-28.679138	3.984745
C	30.520654	-22.844641	4.979786
C	33.355829	-22.935323	9.513285
C	38.878054	-28.645443	8.635549
C	36.504441	-29.704448	1.104653
C	32.460570	-25.714423	3.577374
C	33.836446	-24.526101	7.489245
C	36.902970	-27.527888	7.328759
C	35.864722	-28.300040	3.221270
C	31.363683	-24.765438	3.462061
C	34.078809	-24.070195	8.849499
C	38.065009	-28.401007	7.398392
C	35.603865	-28.782717	1.872053
C	31.407201	-23.989784	4.589261
C	35.063249	-24.875895	9.358756
C	38.240366	-28.905547	6.137691
C	34.399862	-28.253199	1.498971
C	32.515948	-24.489739	5.389742
C	35.425015	-25.799209	8.295539
C	37.167777	-28.357301	5.320989
C	33.956264	-27.427212	2.613714
N	36.378424	-27.530237	6.065599
Fe	34.742217	-26.558850	5.422459
C	33.176224	-31.555442	6.956404
C	34.361006	-32.002591	7.806956
C	32.360069	-27.569922	7.055312
C	33.537718	-27.969746	6.205986
C	33.782730	-29.387887	6.104147
O	34.551711	-29.985068	5.362669
O	32.989634	-30.144051	6.999934
H	29.748675	-22.657799	4.225314
H	31.090841	-21.913470	5.102550
H	30.007016	-23.031734	5.933179

H	30.946285	-24.441476	1.363513
H	29.900216	-25.638985	2.129164
H	29.655068	-23.918352	2.451232
H	33.444117	-27.479205	-0.281215
H	34.202994	-29.061695	-0.490083
H	32.671336	-28.921638	0.381747
H	36.123591	-29.889306	0.094113
H	37.517567	-29.291829	1.003520
H	36.603547	-30.679480	1.601511
H	33.724835	-22.763820	10.530439
H	32.275514	-23.124748	9.584172
H	33.477929	-21.995913	8.956686
H	36.778158	-24.646779	10.657762
H	35.582822	-25.804612	11.243154
H	39.705756	-29.336493	8.442357
H	39.312837	-27.716154	9.029914
H	38.270793	-29.079753	9.442030
H	38.847427	-30.793011	5.281213
H	39.854209	-29.425035	4.798134
H	40.011764	-30.106784	6.422433
H	35.257293	-24.070628	11.352017
H	34.246974	-31.658107	8.839388
H	34.443472	-33.096497	7.814788
H	35.286524	-31.588245	7.404120
H	33.315640	-31.875807	5.920660
H	32.242070	-31.980866	7.338336
H	32.001443	-26.571259	6.814936
H	31.525671	-28.274086	6.963277
H	32.634327	-27.559323	8.122042
H	32.191552	-26.678786	1.706540
H	36.959411	-26.835507	9.332957
H	37.679632	-29.346335	3.520255
H	32.268363	-23.176152	7.033616
S	36.091811	-24.803821	4.476826
C	37.376253	-24.362545	5.708748
H	36.929709	-24.010336	6.645371
H	38.023749	-25.216747	5.937170
H	37.997992	-23.558225	5.298479

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B3LYP Scan/Thiolate IPC Model/Trip/180 degrees Constrained Optimization

C	30.407987	-24.731590	2.323555
C	35.738344	-24.797069	10.713604
C	39.345624	-29.794849	5.638981
C	33.644076	-28.474464	0.249940
N	33.131347	-25.549173	4.772705
N	34.687042	-25.553355	7.191691
N	34.864128	-27.496913	3.662195
C	32.811335	-26.667530	2.624401
C	32.858176	-24.010400	6.660078
C	36.479415	-26.708862	8.387681
C	36.990136	-28.658619	3.996659
C	30.513172	-22.869589	4.991065
C	33.374291	-22.911163	9.510115
C	38.936254	-28.581934	8.634520
C	36.523558	-29.705875	1.124219
C	32.455000	-25.745405	3.603634
C	33.850617	-24.516065	7.496287
C	36.942637	-27.490241	7.334338
C	35.881285	-28.302616	3.241017
C	31.354319	-24.800895	3.485721
C	34.099592	-24.047206	8.850815
C	38.115385	-28.349411	7.400340
C	35.616647	-28.793587	1.895534
C	31.400138	-24.016520	4.606740
C	35.093101	-24.842038	9.359786
C	38.289587	-28.855790	6.140628
C	34.404061	-28.279091	1.528264

C	32.514132	-24.506587	5.406191
C	35.454003	-25.771262	8.301556
C	37.204943	-28.324376	5.328593
C	33.958190	-27.453745	2.642321
N	36.410360	-27.504308	6.074872
Fe	34.756521	-26.560793	5.440028
C	33.045006	-31.584682	6.772818
C	34.099747	-32.121578	7.735331
C	32.413504	-27.576838	7.112925
C	33.570162	-27.977794	6.235626
C	33.805455	-29.396473	6.116757
O	34.668399	-29.981730	5.474986
O	32.893208	-30.172217	6.871866
H	29.738790	-22.689339	4.237439
H	31.082676	-21.936894	5.104986
H	30.002448	-23.049820	5.947347
H	30.930534	-24.496689	1.385695
H	29.884778	-25.685019	2.165944
H	29.643725	-23.960952	2.472333
H	33.444515	-27.519792	-0.256261
H	34.198844	-29.106044	-0.452498
H	32.670283	-28.953816	0.422723
H	36.134842	-29.903108	0.119017
H	37.528726	-29.277694	1.009386
H	36.643957	-30.675976	1.625931
H	33.748086	-22.730143	10.523862
H	32.295384	-23.105549	9.588436
H	33.488496	-21.975344	8.945832
H	36.814745	-24.586105	10.645198
H	35.635952	-25.752937	11.246075
H	39.767321	-29.268771	8.440757
H	39.367002	-27.648013	9.022408
H	38.335526	-29.016094	9.445986
H	38.909546	-30.740427	5.288836
H	39.900753	-29.365177	4.793809
H	40.074301	-30.038359	6.420075
H	35.292532	-24.021952	11.346417
H	33.873151	-31.822415	8.763303
H	34.139249	-33.217232	7.696174
H	35.082005	-31.729293	7.468056
H	33.302729	-31.855606	5.745503
H	32.058308	-31.995861	7.011498
H	32.064500	-26.568930	6.899376
H	31.568234	-28.266967	7.020901
H	32.708016	-27.591542	8.174312
H	32.183388	-26.723530	1.740357
H	37.004810	-26.787417	9.334735
H	37.715355	-29.318014	3.529944
H	32.271089	-23.179796	7.040073
S	36.075216	-24.793683	4.470646
C	37.371898	-24.335717	5.683595
H	36.934046	-23.981823	6.623722
H	38.028445	-25.183797	5.909011
H	37.982400	-23.529007	5.261395

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B3LYP Scan/Thiolate IPC Model/Trip/190 degrees Constrained Optimization

C	30.37552400074897	-24.82170168327459	2.37812709677311
C	35.80032790642730	-24.72954214721927	10.70686261598502
C	39.41854566738399	-29.72907721724983	5.64849940151569
C	33.65092360749248	-28.52758651908759	0.29806852994100
N	33.14250742490680	-25.57009944894265	4.80037968889539
N	34.719012745666281	-25.53574831104660	7.20511831596208
N	34.88678377725841	-27.51005403913421	3.69288322069924
C	32.81474324805173	-26.71403742049458	2.66666512995916
C	32.86893135222768	-24.01720235990512	6.67592136585459
C	36.53458475301878	-26.66012004009592	8.39600055847681
C	37.02789592059345	-28.64659553826016	4.02031319254342

C	30.48440164754274	-22.93096626218145	5.02551287941366
C	33.40600805425146	-22.87924914110441	9.50753127276215
C	39.02035793963223	-28.49368244966562	8.63627990487616
C	36.54931791148873	-29.72265910347006	1.16012999846554
C	32.45547111889938	-25.78831560234173	3.64144838161614
C	33.87609631834182	-24.50252521262633	7.50663828865042
C	36.99663751762580	-27.44633422415514	7.34598746513679
C	35.90871381504186	-28.30955302970132	3.27076832054999
C	31.33837823913767	-24.86259867528688	3.52805667682681
C	34.13455251765627	-24.01611683374378	8.85324508425948
C	38.18327230533362	-28.28683483640044	7.40840571688590
C	35.63869540686384	-28.81406068682215	1.93155847260025
C	31.38555129705639	-24.06648070662523	4.64062279779951
C	35.14053949734151	-24.79604222736609	9.36086110068343
C	38.35228996205861	-28.80273530216107	6.15222973825072
C	34.41804444687691	-28.31464660532739	1.56938271159584
C	32.51704080060222	-24.53109619293469	5.43111548001689
C	35.49891771124272	-25.73392644842095	8.30958856377159
C	37.25078739884100	-28.29610721431641	5.34652879103336
C	33.97180556171304	-27.48548124953243	2.68018165352993
N	36.45170887393454	-27.48012549374136	6.09253164732995
Fe	34.78352197805446	-26.55814924410419	5.46230403195612
C	32.87997634136603	-31.58380019262484	6.50346329154226
C	33.74072856956781	-32.19741567914798	7.60340391126039
C	32.47490051079366	-27.57935667220276	7.18026932635254
C	33.60060586744800	-27.97750918990073	6.26176737313438
C	33.79478675807344	-29.39595628333843	6.08180141748162
O	34.72128172236352	-29.98042370153453	5.53497605417452
O	32.75394500713207	-30.17309949948474	6.64694691425049
H	29.69641275290530	-22.77220631317371	4.28120103474604
H	31.03922880524519	-21.98744563525963	5.12150095848289
H	29.99056358677649	-23.10983830398872	5.99085791725130
H	30.88106748874904	-24.58706726016815	1.43091263630865
H	29.86758331970985	-25.78589196439221	2.23712466204370
H	29.5958527519821	-24.06336062444771	2.52964346170324
H	33.43033828324670	-27.57808945792848	-0.20894989156279
H	34.21106343130349	-29.15133721516151	-0.40712630575586
H	32.68728166376746	-29.02376626800188	0.48021888443188
H	36.15676486417115	-29.92865399999672	0.15817114543107
H	37.54997352612711	-29.28625158243684	1.03736029880385
H	36.68121717932924	-30.68900195008618	1.66622665114098
H	33.78926746845099	-22.68356191450511	10.51502052885971
H	32.32983989797250	-23.08250046298374	9.59997803630921
H	33.50561050899771	-21.948947214711360	8.93153382000708
H	36.87354834098889	-24.50770448518317	10.62409485086593
H	35.71442454810865	-25.68074319097838	11.25049572451923
H	39.85929913248538	-29.17053470540789	8.44120537337158
H	39.44136060412016	-27.54939014434191	9.00952379612015
H	38.43441059489099	-28.92752098850564	9.45867635943136
H	38.99452155949646	-30.68430165789224	5.30990895562376
H	39.95927495198898	-29.29750277340292	4.79495212276401
H	40.15804158231334	-29.95471080834646	6.42484157097900
H	35.35310682495145	-23.95264126484215	11.33645874902864
H	33.34552966462058	-31.94051862188886	8.59111956009584
H	33.76434062212846	-33.29069048583793	7.51568931409128
H	34.76282932607207	-31.82245095182827	7.52968178940760
H	33.30134255459615	-31.81764231658909	5.52234214426927
H	31.85649930528978	-31.97043614492282	6.55285453419193
H	32.13719144575492	-26.56042896863291	7.00429876130171
H	31.61619856453871	-28.25212944526525	7.09492711741993
H	32.80228830568182	-27.62452699136553	8.23148592439061
H	32.17848793853139	-26.78693478435913	1.78985944305123
H	37.07018586700187	-26.72273033047033	9.33850544149487
H	37.75705526873446	-29.30127062158639	3.55309046595012
H	32.27577674630394	-23.18991623418750	7.05374142695243
S	36.07465737834141	-24.78503907959010	4.47027398734230
C	37.38637349023805	-24.31348598265582	5.66170024455219
H	36.9598951685043	-23.95788768047152	6.60644385564619

H	38.05151483321796	-25.15626152963686	5.88169390320195
H	37.98542248074926	-23.50494395959292	5.22680136312363

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B3LYP Scan/Thiolate IPC Model/Trip/200 degrees Constrained Optimization

C	30.36506357050354	-24.85891582531358	2.40739860903992
C	35.84106170990049	-24.68614599798850	10.70311480497449
C	39.46052898429800	-29.68876179163823	5.64932970853419
C	33.64008680626384	-28.56644669618440	0.33508798530557
N	33.14400730158556	-25.58543885978625	4.82318803818602
N	34.73792431065827	-25.52460070364763	7.21577929301876
N	34.89126099055365	-27.52631748919567	3.71750727316359
C	32.81095890202360	-26.74250956663976	2.69725803651282
C	32.87191885600883	-24.02375077183843	6.69139114215775
C	36.57444503124659	-26.62351877250354	8.39812643870422
C	37.04315059921121	-28.64521410157919	4.03655032765849
C	30.47704072359688	-22.95469895180829	5.04461605235206
C	33.42084411214194	-22.86446419611275	9.51183354643586
C	39.07806012192097	-28.43275440364829	8.63048136897379
C	36.54572120302299	-29.74961301897689	1.18832261712788
C	32.45285610280983	-25.81249269955061	3.66835782971305
C	33.88828221375789	-24.49687677269232	7.51772948529265
C	37.03555618970368	-27.41134214342175	7.34902083009051
C	35.91382350989080	-28.32493711076904	3.29424546406131
C	31.33174641855661	-24.89157258559957	3.55442164267859
C	34.15332625223658	-23.99970271805897	8.85908854239988
C	38.22995112999453	-28.24132556773375	7.40775931158968
C	35.63674504894493	-28.83986661600003	1.96048562091952
C	31.37999711678802	-24.08984552353872	4.66283088879902
C	35.17051023837930	-24.76727998556666	9.36324563815021
C	38.39209990650821	-28.76581307500645	6.15459649029733
C	34.41265386040556	-28.34550480683695	1.60186175733999
C	32.51647321186610	-24.54611131057709	5.45112056760413
C	35.52884066498252	-25.70834657128820	8.31487963167941
C	37.27880523958510	-28.27510073388273	5.35506625528713
C	33.97019259424057	-27.51072826034432	2.70952142962914
N	36.48081791403788	-27.45816272610853	6.10080029586043
Fe	34.79806528289025	-26.55729272561596	5.47942007918426
C	32.82365141775009	-31.58267537600435	6.30931028464229
C	33.49416196660596	-32.24013223144056	7.51183351113552
C	32.51045559501033	-27.59552037557132	7.22132071868086
C	33.62811499617843	-27.98488331689795	6.28914721702953
C	33.82455675528173	-29.40215817468468	6.09788183558676
O	34.81715330508609	-29.98927100726852	5.68877204536405
O	32.69691780816495	-30.17378075522227	6.46996125719496
H	29.68550798132142	-22.80271063275284	4.30264041492148
H	31.02959327217722	-22.00903882258317	5.13241629184385
H	29.98775242409861	-23.12894430230843	6.01311670267023
H	30.86692667540948	-24.62705386342382	1.45754170532141
H	29.85940383194501	-25.82513781571957	2.27234133313245
H	29.58749079432991	-24.10203137824188	2.55788429033167
H	33.41590807509640	-27.61975058827026	-0.17554441919948
H	34.19804631342740	-29.19277203621381	-0.36954061429948
H	32.67790973303699	-29.06298085202548	0.52382776087007
H	36.14708678836154	-29.96288576870287	0.19027710111978
H	37.54373080835250	-29.31001398379717	1.05598481246721
H	36.68522919588659	-30.71257884278614	1.69883256050038
H	33.80995728382931	-22.65988064533552	10.51530854987704
H	32.34691533551710	-23.07509300417718	9.61328304496663
H	33.50940479929962	-21.93694042627913	8.92957405526161
H	36.91104933521985	-24.45306321421505	10.61003218703800
H	35.77018016240244	-25.63527722278590	11.25249134492825
H	39.91964219599153	-29.10594719583122	8.43412580364594
H	39.49589164633700	-27.48293226155599	8.99315261350151
H	38.50115153504093	-28.86389864542336	9.46063886856035
H	39.04007287745926	-30.64940407819693	5.32185461148624
H	39.99160633790488	-29.26043333586484	4.78807518055989
H	40.20768832925952	-29.90347363233158	6.42142893560940

H	35.39062270076571	-23.91081460690254	11.33233635565503
H	32.95654465503348	-31.99841874790470	8.43394822261369
H	33.51243252182417	-33.33126848764783	7.39952946462712
H	34.52181560334078	-31.88538771997791	7.60551469607455
H	33.38928015130289	-31.79984651035153	5.39939624294629
H	31.79945898642095	-31.95122489858281	6.18895896716555
H	32.15668831964527	-26.58146423406038	7.04621126067714
H	37.65955543851551	-28.27935385300254	7.15145231339712
H	32.85673847980733	-27.62881562711974	8.26716535650232
H	32.17080963092722	-26.82245152308327	1.82390536112558
H	37.11797403119044	-26.67564306395786	9.33671460173363
H	37.77208433969383	-29.30018392659361	3.56936626739295
H	32.27574408014554	-23.19818006116470	7.06823978144395
S	36.06560545561511	-24.78152290755274	4.46430310470947
C	37.38813092753630	-24.29655736337275	5.63812915866554
H	36.97005065056738	-23.93597026704790	6.58477570939192
H	38.05867102896998	-25.13523625499930	5.85720785918180
H	37.97930430440167	-23.48882008131299	5.19115526922629

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B3LYP Scan/Thiolate IPC Model/Trip/210 degrees Constrained Optimization

C	30.33066288352039	-24.95532000406499	2.46839507936954
C	35.93175761271899	-24.55687831954674	10.67717459635127
C	39.49190960247294	-29.67260753873182	5.69620712209749
C	33.64093853910838	-28.62877318770460	0.39945732178359
N	33.14296872624367	-25.61501761087403	4.86553429837898
N	34.76984201324273	-25.49272384923664	7.23371769822377
N	34.90727548151990	-27.54572128426943	3.76273127198195
C	32.81005936312063	-26.79442746918200	2.75174330881006
C	32.86918596493399	-24.03336883749402	6.71606147813907
C	36.63585120680728	-26.54859439776753	8.40906421502302
C	37.06535310831060	-28.65248671627788	4.08238401636514
C	30.43484778271942	-23.02592186196366	5.08686525006645
C	33.46007619228924	-22.79935598522260	9.49525008614166
C	39.13887235516046	-28.35565902148710	8.65479621548437
C	36.55698098087228	-29.78929929435373	1.24813346464379
C	32.44502412169307	-25.86352633256608	3.71923902363056
C	33.90997993953094	-24.47188675708196	7.53068796953362
C	37.08537415326819	-27.35860105594161	7.37219316765966
C	35.93138902266043	-28.34392808858553	3.34198820635872
C	31.30724547299310	-24.96276648192987	3.60756242554275
C	34.19427826300094	-23.94056633676682	8.85472939265011
C	38.28006410990278	-28.18764003314439	7.43612552461980
C	35.64859241766434	-28.87525911538879	2.01593857303944
C	31.35171588532361	-24.15104957851244	4.70860447908694
C	35.23281202133159	-24.68171963642950	9.35522605296082
C	38.42976802156598	-28.73770348662382	6.19252850249175
C	34.41977727225836	-28.39087696309408	1.65937566383536
C	32.50389651771264	-24.58068079951288	5.48962139713987
C	35.58279493916433	-25.64215103795221	8.32164385865841
C	37.30951728078960	-28.26169747033553	5.39353673515882
C	33.97892055929048	-27.54781234583303	2.76110905095987
N	36.51780681601779	-27.43112275010892	6.13065071507258
Fe	34.82204793108765	-26.55188953722778	5.51325757740403
C	32.70061195199107	-31.52340450991173	5.98343796656387
C	33.16399326757331	-32.33191545133598	7.19141357353779
C	32.61819639524251	-27.61953466057343	7.36197685026057
C	33.67275755455401	-27.98748658352153	6.35132820549250
C	33.82986952483117	-29.39767579144264	6.08149882943839
O	34.83617862333775	-30.00544503415581	5.74594636375891
O	32.63214062305499	-30.12896230254560	6.26469629692029
H	29.62805471959179	-22.90105866704436	4.35627766547230
H	30.97144867447646	-22.06897654512431	5.14866429729926
H	29.96568385605525	-23.19200862408249	6.06660114809882
H	30.82160932600422	-24.72677071260304	1.51205111067097
H	29.83688852171628	-25.92949822149466	2.34754475924713
H	29.54450596767415	-24.20703695095663	2.61735552697305
H	33.40380198302348	-27.68793988973002	-0.11601560749142

H	34.20046274394564	-29.25432289081112	-0.30462649979897
H	32.68509913772675	-29.13370873719521	0.59800699837012
H	36.15514293517054	-30.01178111812661	0.25338423480658
H	37.55351321026675	-29.34872087573621	1.10861041453328
H	36.70040836657665	-30.74774859171766	1.76605967850698
H	33.86264335794854	-22.56997297556839	10.48801121485899
H	32.39010449578595	-23.01852817986416	9.61796931871049
H	33.53002090620577	-21.88335872507908	8.89254672259060
H	36.99225808330629	-24.29546296090648	10.55474419667080
H	35.90078005886059	-25.49690616507934	11.24546800392989
H	39.97663117511289	-29.03542159474486	8.46501108337424
H	39.56278822776078	-27.39969693234301	8.99362154029340
H	38.56828475765135	-28.76746724372199	9.49898831555693
H	39.06493455097466	-30.63473604326265	5.38198696925733
H	40.02336736251018	-29.25833105801476	4.82826741203568
H	40.23978808619354	-29.88192002950727	6.46911102559569
H	35.47389960754560	-23.78276457213041	11.30253660480133
H	32.52218613024002	-32.13910273452127	8.05660878792306
H	33.13504880585017	-33.40686400236870	6.97440876123233
H	34.18862974164857	-32.06027985436855	7.45091305583773
H	33.37208320049006	-31.69373029963969	5.13813313933517
H	31.68380868465620	-31.80904716508402	5.69431100194624
H	32.18624949769262	-26.63588988502285	7.17474301334796
H	31.80852882079822	-28.35337937443718	7.40328582236869
H	33.06252788243867	-27.57264494334050	8.36910998357602
H	32.16367312124231	-26.89106813523618	1.88473311318344
H	37.19274353818744	-26.57691614783534	9.34084270064523
H	37.79210852112572	-29.31354306793538	3.62047639155791
H	32.26513719526471	-23.21161154769500	7.08883027542237
S	36.05148748408818	-24.77763636936022	4.46225926087908
C	37.39364530210285	-24.27294790044315	5.60487538568395
H	36.99159452283407	-23.89660877086832	6.55237287784259
H	38.06797642199635	-25.10779077231757	5.82641984060596
H	37.97660151837794	-23.47262020598252	5.13438562961322

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B3LYP Scan/Thiolate IPC Model/Trip/220 degrees Constrained Optimization

C	30.30926037770375	-25.04333281008701	2.52010374724651
C	36.00927243311476	-24.46899102479807	10.65533790991188
C	39.53874943157778	-29.65368990220074	5.72256638866604
C	33.66040002618977	-28.67258485905808	0.43909953546299
N	33.15336782407253	-25.64474254903481	4.89511663372805
N	34.80394754741617	-25.47915384984054	7.24751284829837
N	34.93032503552504	-27.56756751226089	3.79411470972526
C	32.82644343050322	-26.83191175383039	2.78473870887672
C	32.86175234082641	-24.06896114253845	6.74763725933632
C	36.70390548192023	-26.48927489706834	8.40903124179264
C	37.08665800860707	-28.67674549526317	4.11987257212184
C	30.38739857102968	-23.11975339801446	5.14399910530785
C	33.47223244080492	-22.79018457210041	9.50208532167743
C	39.22599419495820	-28.26744797182635	8.65346068401952
C	36.57409090752203	-29.83343634336945	1.29530886065786
C	32.45262054497093	-25.90596407387190	3.75339939352583
C	33.92507879661076	-24.47594605524959	7.54901086952045
C	37.14245501572385	-27.31793243716983	7.38273750277557
C	35.95213434144393	-28.37188213873632	3.37869832548877
C	31.29467310669459	-25.03011852198279	3.65161602429678
C	34.21980363667007	-23.92268828431389	8.86153885187751
C	38.34395297115339	-28.13721210411688	7.44665971876434
C	35.66772739071891	-28.91221256010461	2.05698838524618
C	31.32788763911893	-24.22150212895421	4.75517380562759
C	35.28545494026591	-24.63223061803226	9.35101753610318
C	38.47642043665278	-28.71670490503251	6.21472582377562
C	34.43995935257954	-28.42727237853186	1.69716809777092
C	32.49606954558282	-24.62650628813700	5.52611695935236
C	35.63781255080303	-25.59804147595259	8.32330432831887
C	37.34100955806763	-28.26506192119702	5.42257821469596
C	34.00028734681808	-27.57719922683403	2.79359949269606

N	36.55503377494308	-27.42232732417807	6.15239730048478
Fe	34.85058750760482	-26.55454912776492	5.53502708323974
C	32.54986887356510	-31.42483600416164	5.73718103561505
C	32.81820373838850	-32.28744240942554	6.96637630498227
C	32.71248481967704	-27.64175900730340	7.45956540384570
C	33.70651986822934	-27.99294854540942	6.38456909502121
C	33.80429003371240	-29.39192673281003	6.03910138899054
O	34.80047959112948	-30.05230520047680	5.78650983531549
O	32.54597363654072	-30.03377838594307	6.04805249929607
H	29.56203766621163	-23.02439594056499	4.42986005361281
H	30.89730492125916	-22.14715824151540	5.18687047438963
H	29.94449762792235	-23.29135848348848	6.13481118966738
H	30.78790343088077	-24.80485266140472	1.55996330409858
H	29.83518910682703	-26.02768313545471	2.40327816149136
H	29.50908849499548	-24.31133756138120	2.67515193259584
H	33.41859988539458	-27.73432746014530	-0.07876267107699
H	34.22179799490237	-29.29781479549784	-0.26377916865802
H	32.70707032958487	-29.18111504243405	0.64049141676191
H	36.17202668533593	-30.06110971637680	0.30184570561663
H	37.57177341387442	-29.39626928483800	1.15324444915531
H	36.71493976031982	-30.78892787927021	1.81931756785535
H	33.87467088013479	-22.55376251155793	10.49325724761855
H	32.40577134052577	-23.02342026295438	9.62837928951501
H	33.52823672297495	-21.87413003587476	8.89789528648109
H	37.04792905795532	-24.14057071017987	10.50787667623485
H	36.05168831738024	-25.41095822792103	11.21926811056920
H	40.06357689148679	-28.94825546944840	8.46674975093329
H	39.65120378810421	-27.30037561514200	8.95737723320150
H	38.67381162654645	-28.65815472592185	9.51955635396018
H	39.11383590464055	-30.62110255948930	5.42234188683088
H	40.06345682583324	-29.24773516604993	4.84650285308438
H	40.29230140639696	-29.85104130904427	6.49313676874744
H	35.52016860674505	-23.72742622951828	11.29631282630882
H	32.09834287408110	-32.06574881185914	7.76031151771608
H	32.73906916296335	-33.35314633126551	6.71856299989594
H	33.82354142256362	-32.09561360894558	7.34517717043627
H	33.29808872800336	-31.62469255056257	4.96608818075088
H	31.55466376201143	-31.63055392654368	5.33008940655717
H	32.11479801005211	-26.76212613152136	7.19947531027751
H	32.02659728185545	-28.46369765574451	7.68437137043228
H	33.23957386191524	-27.37813311526424	8.38755579860662
H	32.17746040254011	-26.93816837368905	1.92085651134017
H	37.27676963674325	-26.49309570738596	9.33149245644757
H	37.81036353839617	-29.34460627381869	3.66303969931731
H	32.24283793267875	-23.26042432237024	7.12501080671588
S	36.05399390217293	-24.78081523640997	4.46243700123944
C	37.41391873248100	-24.26382966340830	5.57786924027664
H	37.02713460891323	-23.87629765311286	6.52726649815660
H	38.09188939203225	-25.09590639597617	5.79840994750378
H	37.98897399492702	-23.46901227966722	5.08865758187876

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B3LYP Scan/Thiolate IPC Model/Trip/230 degrees Constrained Optimization

C	30.28437542682842	-25.10858264091299	2.56931093834226
C	36.06555915194118	-24.39448844184457	10.63712659884600
C	39.55436605237873	-29.65227926899847	5.75090206444496
C	33.64539120680737	-28.72704064462113	0.49019278092204
N	33.15659899439061	-25.66088684976848	4.92281945724444
N	34.82614507582248	-25.46005734264899	7.25841485747590
N	34.93596175271468	-27.58681206350129	3.82549823758663
C	32.82219334163280	-26.86783588782319	2.82441592388244
C	32.86571617014180	-24.07296412161845	6.76477482233852
C	36.74603019946408	-26.44212914675403	8.41114303309193
C	37.09350827491783	-28.69325458409132	4.15165884308600
C	30.36317065332435	-23.16686656481003	5.17970482621391
C	33.49914829878966	-22.75337154157930	9.49459311263798
C	39.26848819414237	-28.21926942061918	8.66173976315803
C	36.56392900533837	-29.88030527998416	1.34093130263121

C	32.44854975130939	-25.93799420530215	3.78923426257392
C	33.94215741427336	-24.46078947298925	7.55813488788523
C	37.17708746737490	-27.28445261210111	7.39281895958489
C	35.96504602009704	-28.39641178972555	3.41271914352202
C	31.27997330610124	-25.07580344633995	3.69153568813658
C	34.24833273925627	-23.88804647645001	8.85974783069602
C	38.37778183060651	-28.10474503018538	7.45973791566988
C	35.66220659784311	-28.95140139624975	2.09897464050691
C	31.31347179662014	-24.25958093435804	4.78928906772065
C	35.32622631835756	-24.58181915068201	9.34475138685600
C	38.49899634105870	-28.70398699055689	6.23626165982002
C	34.43239374828684	-28.46930956603025	1.74124541485405
C	32.49334568429152	-24.64586607152135	5.55223052373451
C	35.67375404863515	-25.55832493197647	8.32540785434205
C	37.35843187011725	-28.26177776144023	5.44606639047772
C	33.99917637129077	-27.60806446096273	2.83116986758903
N	36.58044542350835	-27.40535153135526	6.16851069445636
Fe	34.86805053264511	-26.54965737115975	5.55567071760335
C	32.54626972180382	-31.34630822285768	5.51423866681975
C	32.56714177251938	-32.26129222901651	6.73389374981600
C	32.77154388282132	-27.66897077763369	7.52955126254885
C	33.74143498173971	-27.99098505801187	6.42450777730413
C	33.83833321469095	-29.38727387602474	6.05860533739198
O	34.83300132708876	-30.08176236715221	5.93173724514623
O	32.56661059146464	-29.96758180817572	5.87945375879257
H	29.53093042341493	-23.08532026454668	4.47184312396425
H	30.86176498142983	-22.18802224898266	5.21303383220450
H	29.93063978307430	-23.33826767580560	6.17511793464372
H	30.75221290539314	-24.87563399001803	1.60251009373041
H	29.81765385331717	-26.09797929179445	2.46655452294066
H	29.47955465375678	-24.38173106738224	2.72452428654258
H	33.40937510191437	-27.79471156829592	-0.04093582190415
H	34.19827187075266	-29.36778040003540	-0.20541291523277
H	32.68856744614906	-29.22393497550506	0.70341317356765
H	36.15333267492156	-30.12140822496199	0.35414505864114
H	37.55923354425502	-29.44278548917132	1.18410072128097
H	36.71214829342177	-30.82884604415641	1.87542870544240
H	33.91057093281664	-22.50187352266463	10.47834389505136
H	32.43592441749079	-22.99296547801387	9.63541030187092
H	33.54164211021669	-21.84441564707544	8.87869785920289
H	37.09744839039330	-24.05343769435255	10.47189785556104
H	36.12877726343630	-25.32943668393291	11.21071721364779
H	40.10470976008074	-28.90247186652986	8.47776551986779
H	39.69581688352870	-27.24842172935681	8.95023895266665
H	38.72249443010825	-28.59897226673973	9.53658848254253
H	39.12377235357239	-30.62333760249861	5.47123357688064
H	40.07268509992669	-29.26318348111268	4.86346557848662
H	40.31405106969655	-29.83875681037556	6.51815154219135
H	35.57495028089468	-23.65264823909778	11.27665257857999
H	31.74347557739246	-32.02084343576236	7.41309909432823
H	32.47129712006051	-33.31222628827035	6.43449483417816
H	33.50814585881610	-32.14211532031897	7.27427190675166
H	33.39768599536226	-31.56344712103052	4.86472464692270
H	31.62099708599857	-31.47930922915977	4.94463853023604
H	32.21607302546194	-26.74498560207316	7.34294937962634
H	32.04537104065501	-28.47230232136704	7.69575261728704
H	33.31326290556916	-27.50879799701801	8.47419855567080
H	32.16699433866893	-26.98555755026692	1.96674696292716
H	37.32806180931328	-26.43091303927527	9.32779587277621
H	37.81297616562033	-29.36913112826016	3.69992989301031
H	32.24257217890463	-23.26695746401252	7.14065634276075
S	36.05184894367154	-24.78239608961219	4.45515718741547
C	37.42437128860701	-24.25390620109143	5.54932826536496
H	37.04881960379220	-23.85169719145732	6.49717349670784
H	38.10205906029827	-25.08489007134089	5.77453132348069
H	37.99659992540892	-23.46775734944313	5.04306075243381

B3LYP Scan/Thiolate IPC Model/Trip/240 degrees Constrained Optimization

C	30.27097170186181	-25.12040759233400	2.58968148488198
C	36.09908790561649	-24.35333236309091	10.62014214052108
C	39.53599178332669	-29.67668249159066	5.76919939654156
C	33.62546075679055	-28.74305044788443	0.50982664534452
N	33.15306866374078	-25.66082669955184	4.93387287043834
N	34.83234735779288	-25.44898433687039	7.26108573687527
N	34.92481766348907	-27.59856115895839	3.84019753496045
C	32.81228217867503	-26.87437895855737	2.84005026441553
C	32.86817229172421	-24.06630044031293	6.77081734340158
C	36.75894443354579	-26.42323569478853	8.40929692102345
C	37.07604759465757	-28.71645071492941	4.16975488428900
C	30.35325153653793	-23.17484695359749	5.19728154091978
C	33.52473260591388	-22.72041091792275	9.48234206661328
C	39.27239981475262	-28.21160762346592	8.66598791668374
C	36.53788809612195	-29.91043534039520	1.36263515123721
C	32.44110287165741	-25.94272542841667	3.80400378015985
C	33.95150495342719	-24.44616325882595	7.55862377761713
C	37.18125320174920	-27.27675455304640	7.39665909599088
C	35.93866446577901	-28.41637164547237	3.42995532658761
C	31.27001999912450	-25.08338721938686	3.70870322148728
C	34.26835607071381	-23.86153679893044	8.85242989671574
C	38.37735993920405	-28.10344364633008	7.46660764108834
C	35.64128959937697	-28.97498091081640	2.11886890425143
C	31.30523419361166	-24.26536892810566	4.80490699959355
C	35.34950113347517	-24.55159974183115	9.33527414606297
C	38.48915013304523	-28.71631957814824	6.24913234155838
C	34.41415906990860	-28.48619428042247	1.76003592616529
C	32.48951699830689	-24.64672050249128	5.56369165668770
C	35.68784462298481	-25.53816246444362	8.32247380019407
C	37.34798975722917	-28.27479368400785	5.45939579973688
C	33.98673849461810	-27.61859585759244	2.84692162382933
N	36.57853049339813	-27.40572569341247	6.17611029804504
Fe	34.86669519079398	-26.54650660542555	5.56390094440576
C	32.57871385293012	-31.31315560262125	5.40057653777809
C	32.51334682306561	-32.23054561547525	6.61658607136284
C	32.81935634112734	-27.69675030270201	7.59498668602166
C	33.74126720348531	-27.98493315990757	6.44107126983907
C	33.84898776200097	-29.38417551094057	6.07449158579809
O	34.83407365351646	-30.10119374853215	6.05714308225201
C	32.59258786684473	-29.93225500200575	5.76498063287666
H	29.51961222510954	-23.09489164019034	4.49088274972993
H	30.84966651499626	-22.19487062976327	5.23006256427631
H	29.92299021976037	-23.34758956200728	6.19346726729636
H	30.73537388910306	-24.88817875842913	1.62103140325546
H	29.80616625035523	-26.11101514666948	2.49011434974877
H	29.46507716901657	-24.39497159093028	2.74599997242387
H	33.39714881552919	-27.81117034009054	-0.02543740977418
H	34.17337676533374	-29.39125479958712	-0.18279509265216
H	32.66461392824275	-29.23121808407398	0.72495495425807
H	36.12421052955059	-30.15404344367550	0.37774991044125
H	37.53434753858118	-29.47700214437434	1.20178333977511
H	36.68436029260544	-30.85751708721471	1.9002377299560
H	33.94642401988890	-22.45736950918737	10.45870653971352
H	32.46333651150680	-22.95949819028283	9.63730733049741
H	33.55951047871719	-21.81854822348841	8.85568787336280
H	37.13205044332458	-24.02152339514058	10.44344003161325
H	36.16015056841717	-25.28141900582346	11.20512326780352
H	40.10701770231700	-28.89706142418391	8.48316936557275
H	39.70194604832292	-27.23951649898085	8.94683624839160
H	38.72918535297627	-28.58524552894794	9.54518019405630
H	39.09856101963636	-30.64951461376355	5.50672344159186
H	40.04935218376486	-29.30278956293960	4.87242177450764
H	40.30064330876989	-29.85603289132885	6.53321367090213
H	35.61793193923466	-23.60015583159812	11.25357791771022
H	31.65030205276717	-31.98433876857708	7.24295763573994
H	32.42662614922665	-33.27950206298118	6.30776345861324
H	33.41943858327915	-32.12207061275009	7.21510730376863

H	33.46514976227224	-31.54001114623634	4.80308861297179
H	31.68896548389143	-31.43285244127688	4.77461225704071
H	32.32858668883504	-26.72368447114298	7.50865430796429
H	32.03833678656184	-28.46034916695292	7.70090668450787
H	33.38292950089539	-27.67348574010335	8.54175593634774
H	32.15502732465267	-26.99313672887950	1.98409772115763
H	37.34663486136500	-26.40483749757268	9.32221727407936
H	37.78967858856541	-29.40120955062901	3.72214660076125
H	32.24623212555604	-23.25879538929141	7.14552875139170
S	36.04921172379573	-24.78786584866946	4.44924587111428
C	37.43191800699304	-24.26041026947997	5.53112666331991
H	37.06499811331098	-23.84988142974061	6.47881189931033
H	38.10625855716252	-25.09381575451873	5.75726154551697
H	38.00542789988715	-23.48076074498631	5.01629209464461

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B3LYP Scan/Thiolate IPC Model/Trip/250 degrees Constrained Optimization

C	30.26128072017739	-25.07444486683853	2.60916717037654
C	36.10794303306098	-24.34444047907542	10.62734924789760
C	39.48467146566070	-29.71596175565370	5.77983992509959
C	33.53305357248281	-28.78845135704023	0.56560847266687
N	33.14293712247877	-25.63470985991786	4.94981614539506
N	34.83297938491054	-25.42563831344472	7.26634555304166
N	34.88908764945732	-27.59866249988546	3.85694557348368
C	32.77636305421453	-26.86275014858685	2.86785989092474
C	32.87659260729434	-24.03048878907881	6.78077764088927
C	36.76233643189151	-26.40484017257767	8.40560086155053
C	37.02585174643760	-28.74401186168801	4.18721890391226
C	30.37563629534155	-23.11085240863436	5.20159727195925
C	33.53587790587788	-22.70199942560667	9.49975908438998
C	39.25962372115833	-28.21483336822686	8.66109369265839
C	36.43648587431265	-29.98595580182977	1.40788997666894
C	32.42400044873935	-25.91604481224126	3.82394482516982
C	33.95598667926990	-24.42114593314013	7.56871442810389
C	37.17687939606644	-27.26167502005235	7.39252256578764
C	35.88509141865153	-28.44107286495231	3.45224617171942
C	31.26390275752983	-25.04234056055857	3.72514920292817
C	34.27627038844936	-23.84214915962563	8.86440712160961
C	38.36299543087380	-28.10237477880976	7.46350402431065
C	35.56371659360850	-29.02147063234998	2.15583540037784
C	31.31200774541856	-24.21707356930459	4.81549745648047
C	35.35671236604343	-24.53614185477055	9.34255849665855
C	38.45890123015392	-28.72988533807635	6.25257752794344
C	34.34086180192546	-28.51913588350079	1.80097107943228
C	32.49259675810843	-24.60867386751841	5.57442907420942
C	35.69126313441291	-25.51979515273535	8.32544287839561
C	37.31925063024111	-28.28087891557425	5.46494482467870
C	33.93972037542834	-27.62395310988694	2.87540541189157
N	36.56805724125478	-27.39122876162162	6.17589368007767
Fe	34.85753369035253	-26.52551331257379	5.57301838487311
C	32.96383098104504	-31.35986346394704	5.28085613931577
C	32.57090785247213	-32.24404262799065	6.45899918250555
C	32.72663559959619	-27.68938295434496	7.52350415293128
C	33.75818426876012	-27.96990018519745	6.46555085578425
C	33.98272401116812	-29.38267579074168	6.19639494147446
O	34.95636766514259	-30.06607140883996	6.45490569309299
O	32.86355718621110	-29.96871434811747	5.59606360537104
H	29.54048354576438	-23.02638026275926	4.49752448572900
H	30.88486082229444	-22.13718050053910	5.22371330315465
H	29.94656051794492	-23.26876996313172	6.20074897225040
H	30.72570703629536	-24.85538762044766	1.63750308733572
H	29.78311292926996	-26.05956067822748	2.51820206076108
H	29.46519843079744	-24.33758089182724	2.76242582282149
H	33.31438469872129	-27.86421769523638	0.01326941424282
H	34.06132208265853	-29.46063457694415	-0.11936185163886
H	32.56642434056428	-29.25461980195665	0.80241919919555
H	36.00557158615424	-30.24443768831052	0.43423600263194
H	37.43671290721200	-29.57072035606955	1.22404849569035

H	36.57766372869644	-30.92374653189293	1.96309969473474
H	33.95245333615794	-22.45061002450124	10.48137193727887
H	32.47193832972042	-22.93559658842936	9.64494329585958
H	33.58083375935421	-21.79442573590046	8.88186341029394
H	37.13733831594627	-24.00092243153055	10.45185468246432
H	36.17890774389357	-25.27824517064237	11.20178896399738
H	40.08901553837032	-28.90648401183788	8.47787498769600
H	39.69638038295006	-27.24537934415939	8.93981426433809
H	38.71496574361333	-28.58375479013359	9.54135141420205
H	39.02873502966232	-30.68798465274565	5.54712517409328
H	39.99052843547550	-29.37116662465618	4.86735490596745
H	40.25733220741051	-29.88924132428992	6.53711175785825
H	35.62140178234633	-23.60266082847306	11.27010679407912
H	31.56538570844383	-31.99558774184153	6.81213458446638
H	32.58197737485530	-33.30236174341582	6.17125418473069
H	33.27287853344184	-32.10513258939475	7.28334404922189
H	33.98347380743468	-31.58485394123755	4.96034392567406
H	32.28383993078540	-31.50913698287595	4.43682690709301
H	32.25970619827077	-26.70897158057257	7.40523293148663
H	31.92675623036333	-28.44377803774886	7.52761927018116
H	33.18002164391041	-27.69840899949370	8.52960086672193
H	32.11032978511098	-26.98308222193108	2.01889244232240
H	37.35293467925789	-26.38945187340454	9.31667520435772
H	37.72459872084829	-29.44791681511040	3.74570976191752
H	32.26203195609666	-23.21742686544566	7.15554988539199
S	36.04592020821477	-24.79262033620779	4.42927644452082
C	37.41897094050440	-24.24669839903532	5.51431000511263
H	37.04406737974736	-23.82498741293796	6.45384894136549
H	38.09361139964351	-25.07546903973462	5.75593285657768
H	37.99447103611576	-23.47243891041334	4.99356792778328

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B3LYP Scan/Thiolate IPC Model/Trip/260 degrees Constrained Optimization

C	30.25088139919718	-25.04108662272004	2.62065074247858
C	36.11917963151277	-24.34189079545281	10.62514750801179
C	39.44894771685161	-29.74436828144830	5.77679646857360
C	33.47740502829479	-28.79617828760293	0.58463046366176
N	33.13436845516423	-25.61695632596387	4.95517010969361
N	34.83577715831857	-25.41019076237767	7.26293741487602
N	34.85863900564578	-27.60111795903939	3.86381017940148
C	32.75178367433547	-26.84753642886350	2.87717709721554
C	32.88027075020462	-24.01091787932641	6.78639957964199
C	36.76957781924026	-26.39138458657685	8.39349085573867
C	36.98051451230660	-28.77368361339337	4.19659776099762
C	30.38078861128479	-23.07872200534427	5.21368799895125
C	33.54239952798395	-22.69753989494398	9.51229748357862
C	39.26092136478530	-28.21004578528748	8.64269604190971
C	36.36712165156489	-30.02653783327374	1.42713164858521
C	32.41060666992762	-25.89500222840076	3.83136423383719
C	33.96009308417596	-24.40664486037745	7.57137604391058
C	37.17359300666206	-27.25563137484714	7.38276181135248
C	35.84026559008353	-28.46172460302004	3.46352951017894
C	31.25606620230179	-25.01408451399125	3.73444907352437
C	34.28374687519452	-23.83228606277555	8.86863762582105
C	38.35468764933944	-28.10322549528806	7.45190148233727
C	35.50751479717176	-29.04806280276467	2.17226781240587
C	31.31120771667372	-24.18887231023420	4.82454040375057
C	35.36631860612731	-24.52679329904501	9.34040705850714
C	38.43442462004721	-28.74584626295568	6.24779378029349
C	34.29135715770833	-28.53071293420014	1.81679972366719
C	32.49124768623066	-24.58662149001051	5.58058380986002
C	35.69813076440719	-25.50680064491406	8.31875098203719
C	37.29091702065683	-28.29709745389235	5.46571362779489
C	33.90600955819383	-27.62210505602886	2.88617762548041
N	36.55374304859527	-27.39218817981013	6.17257155290554
Fe	34.84548772660417	-26.51516237573007	5.57323086261476
C	33.28639167350995	-31.40443739231778	5.28007440311300
C	32.59013077156892	-32.24417510664291	6.34463918210535

C	32.65464996560053	-27.68780480659456	7.47896105043626
C	33.74961235401060	-27.95537084797412	6.48352556636634
C	34.05356092572642	-29.37333063742795	6.31498007868266
O	34.96434464853381	-30.01585559926752	6.80213319643383
O	33.10561552133890	-30.00366629910243	5.51073205097477
H	29.54505967260630	-22.98922508762200	4.51095974238396
H	30.89457164673936	-22.10749964505288	5.23679529563588
H	29.95244577901000	-23.23648256086409	6.21318781621347
H	30.71475487068136	-24.82582188160933	1.64787666630279
H	29.76651262441357	-26.02335210023401	2.53145628337976
H	29.45958409249999	-24.29925589295447	2.77471255348385
H	33.27351023869818	-27.87288258306670	0.02501522669939
H	33.99348037256003	-29.48255881732917	-0.09556198096376
H	32.50346095511905	-29.24406876223098	0.82648719416918
H	35.92804157368064	-30.28892534903447	0.45816600879130
H	37.36978346194903	-29.62145474482756	1.23381869920226
H	36.50400220808194	-30.96130076227421	1.98849774920435
H	33.95455599484151	-22.45748641037567	10.49860541408500
H	32.47747096527727	-22.93111762666911	9.64977231066436
H	33.59167780781385	-21.78320041019558	8.90467108997140
H	37.14482945786656	-23.98635150266654	10.45141321713054
H	36.20025959563882	-25.28160080063208	11.18833472475211
H	40.08890024637743	-28.90250867443777	8.45606572255857
H	39.69978751922221	-27.23939236079481	8.91356656046107
H	38.72294610565211	-28.57538990056999	9.52847098664454
H	38.98595812661508	-30.71824736157530	5.56635184580881
H	39.94376205145183	-29.41696901684251	4.85197001796132
H	40.23114323554917	-29.90899955074871	6.52611616039704
H	35.62700904577128	-23.61238628547089	11.27761543317032
H	31.53024324582106	-31.98107156746950	6.41296713434754
H	32.66369887764648	-33.31274563352411	6.10885031516021
H	33.05204439775856	-32.07581553965399	7.31968018239823
H	34.35443751590499	-31.63027781161146	5.25338282416614
H	32.85651316189627	-31.58963652660085	4.29142822108081
H	32.27744627922208	-26.66600649741167	7.42196784353445
H	31.79881976818072	-28.36698464938451	7.33515343921967
H	33.00152053151854	-27.84123425315062	8.51652075621201
H	32.08254520001018	-26.96404833910471	2.03017361254644
H	37.36599322768011	-26.37424820360984	9.30070109047959
H	37.66842492938092	-29.48978044958544	3.75747957486946
H	32.26923867382786	-23.19649395532988	7.16390339234398
S	36.04499425718321	-24.80494228764985	4.41317881399051
C	37.41195758046469	-24.24534039327784	5.49871011585008
H	37.03264998245757	-23.81375975463216	6.43187987161885
H	38.08661695644373	-25.07051558085024	5.75228999112703
H	37.98853281940443	-23.47623776984720	4.97156118124096

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B3LYP Scan/Thiolate IPC Model/Trip/270 degrees	Constrained Optimization		
C	30.21008094106652	-25.04081640927516	2.68021455783180
C	36.18382693097708	-24.27278247431243	10.60036553025090
C	39.37882476842353	-29.81816367043415	5.82547504455819
C	33.39556209289560	-28.83387548486360	0.64661281136328
N	33.11611094493351	-25.61032354967995	4.98856712958240
N	34.84303300310145	-25.38565507183008	7.27434266030308
N	34.81256017140635	-27.61778021838008	3.90271279333586
C	32.70689343417218	-26.85436341632078	2.92350628945944
C	32.89196982719550	-23.98013277682766	6.80343896946673
C	36.78290879087788	-26.36527874728066	8.39741484253356
C	36.90802165921335	-28.83533591609217	4.24798002070321
C	30.37826344884399	-23.05610586100392	5.25428210936748
C	33.60020181677401	-22.62933608683941	9.50035853869054
C	39.25343007448919	-28.21189637526840	8.65498614967222
C	36.27039432439710	-30.09973321086952	1.49203001047548
C	32.37945332526041	-25.89334924341883	3.87373472356089
C	33.97937729692903	-24.37145175734600	7.58035714438376
C	37.16173076560440	-27.25814204562645	7.40187341543402
C	35.77509631760898	-28.50283575470317	3.51199796575534

C	31.22856887929052	-25.00768601087664	3.78164379066947
C	34.32563493403773	-23.77846944407170	8.86395701173211
C	38.33127403852913	-28.12103722848876	7.47507143095508
C	35.42810795300043	-29.09989820133960	2.22884435229130
C	31.30007271805070	-24.17292278140615	4.86362723789623
C	35.41048837098428	-24.47257913701401	9.33000449711346
C	38.38423496920142	-28.79483594327476	6.28604705331177
C	33.85488813284605	-28.56655295350243	1.87142283071145
C	32.48616172101802	-24.56906454455612	5.61006375843402
C	35.71933403920808	-25.47229768443720	8.31965804016787
C	37.23820435158919	-28.34583347769103	5.50800310393691
C	33.85488813284605	-27.63797839944096	2.93126258590402
N	36.52346743517251	-27.41444344207705	6.20372117719774
Fe	34.82147404170678	-26.51714530647036	5.59874668166227
C	33.70046139956864	-31.36122735581488	5.17683062726982
C	32.77512817147893	-32.25118987238746	5.99827895698759
C	32.50400282311028	-27.66232891552028	7.37759779544965
C	33.73747511405724	-27.94000707700017	6.56277687879636
C	34.05147403390657	-29.36538365403377	6.46114645794370
O	34.75221238476274	-30.02247691061108	7.20939089396285
O	33.42200447404191	-29.97173508315331	5.38438084134465
H	29.53488325335529	-22.96919146407678	4.56050427742775
H	30.89562582041728	-22.08658195243245	5.26382612114717
H	29.96099746656540	-23.20457647051209	6.25983307807980
H	30.66227015564892	-24.83342584850331	1.70025903340056
H	29.72300443213510	-26.02283700541638	2.60415907188124
H	29.42180734388312	-24.29669781839329	2.83865227700579
H	33.19779261819466	-27.91334629849939	0.08034579490878
H	33.90011792886393	-29.53151805350084	-0.03076948368146
H	32.41852276799580	-29.26941709651697	0.89854297000586
H	35.81892339280507	-30.37389783717824	0.53206880736457
H	37.27516562614840	-29.70820619102495	1.28218370084061
H	36.40355486179626	-31.02626168238969	2.06776140608193
H	34.03340671710809	-22.37122109478954	10.47299522174155
H	32.53784863502095	-22.85751933662038	9.66439723139290
H	33.63873927593809	-21.72724952336056	8.87396797255734
H	37.21177784169589	-23.93577645960757	10.40480099930626
H	36.25971853357299	-25.20182036324064	11.18168041191003
H	40.07685514857504	-28.90978592140790	8.46842257469138
H	39.69854920132803	-27.23821886971349	8.90347560664523
H	38.72668195314981	-28.56097369078611	9.55389487191462
H	38.90324447434816	-30.79374976203767	5.65363551974126
H	39.85805829956808	-29.52387690895418	4.88162204223159
H	40.17414321030218	-29.96809434891693	6.56389181109782
H	35.71133138765111	-23.52286248921276	11.24418384871286
H	31.72716562249749	-32.01514729549235	5.79026392615080
H	32.94194524620279	-33.30932857277219	5.76324077621368
H	32.95902552790812	-32.10226503682452	7.06381727684800
H	34.74510104112404	-31.56012773758896	5.42582551449008
H	33.55311506513335	-31.52041442308690	4.10524370246411
H	32.38082254105602	-26.60294223895777	7.60298589318754
H	31.58529036251992	-27.98973027473262	6.85787695240044
H	32.52346624659289	-28.20410309190657	8.33842523774319
H	32.02948674972110	-26.97357167990553	2.08339316169023
H	37.39152727995995	-26.33593106572098	9.29612467956101
H	37.57898752110098	-29.57088411626325	3.81459589248983
H	32.28991805331023	-23.15740128916112	7.17726448275277
S	36.04440871557982	-24.85775252285022	4.39607690862336
C	37.39909814328148	-24.25916935894665	5.47618763000826
H	37.01062126766735	-23.79720638401005	6.39063728915705
H	38.07262303201651	-25.07426047072099	5.76314555917339
H	37.97959606928714	-23.50748346042754	4.92855024017426

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B3LYP Scan/Thiolate IPC Model/Trip/280 degrees Constrained Optimization

C	30.21180929619048	-25.01764944423150	2.65357996740629
C	36.15933510083144	-24.28747747853232	10.59726754721533
C	39.35313482943402	-29.83135854939540	5.82038665058655

C	33.39285931885901	-28.81556346205418	0.62313471198879
N	33.10555066241517	-25.60301312595414	4.97304878358418
N	34.82560176796718	-25.39093539662701	7.26535929585169
N	34.80099617237062	-27.61280079284738	3.88801732521872
C	32.70118422140096	-26.84028482290885	2.90325727209742
C	32.88238168332834	-23.97540713920113	6.78962124676460
C	36.75558034955525	-26.38234654818464	8.39566943757805
C	36.89263529707488	-28.83532059390928	4.23659311579150
C	30.37541648189166	-23.03991223192714	5.23336935044194
C	33.58966749352445	-22.62863964320453	9.48742334493133
C	39.21678655130707	-28.24075106108149	8.65841229231398
C	36.26254283005024	-30.08909988730257	1.47401361401625
C	32.37266223850120	-25.88111887951058	3.85485284524162
C	33.96643173473898	-24.37163921823215	7.56838852497415
C	37.13564525451214	-27.27308798541059	7.39880607755522
C	35.76298059564464	-28.49817612101245	3.49760007249340
C	31.22500490476439	-24.99128648012725	3.76003866749172
C	34.31114692907692	-23.78146218549445	8.85321937030308
C	38.30171011073860	-28.14041566837424	7.47384367948912
C	35.41942383424622	-29.09026969129465	2.21128041509983
C	31.29436696649067	-24.15965390328023	4.84442655053365
C	35.38992204168946	-24.48228909031763	9.32375626133400
C	38.35886790999875	-28.80802206044873	6.28162657409697
C	34.21331311271135	-28.55350326263988	1.85163487630603
C	32.47648814203997	-24.56167671888375	5.59465331486730
C	35.69734784903410	-25.48295854764685	8.31425735908328
C	37.21812436459124	-28.35175069783665	5.50000111244826
C	33.84647244344267	-27.62776632696590	2.91344899549389
N	36.50241487147741	-27.42169241145727	6.19685184395875
Fe	34.80607074314693	-26.51735992597921	5.58828342784043
C	33.72929847472933	-31.36410423992018	5.17255976671746
C	32.81428781649552	-32.27057692370313	5.98732096294023
C	32.62980339155087	-27.64546710253432	7.54845838030212
C	33.70867460921508	-27.93878161664730	6.54050569825978
C	34.03649051838712	-29.36180595578160	6.45484457237284
O	34.74973512471146	-30.00352152393694	7.20579216050299
O	33.42288638597218	-29.97995179947731	5.37782070848721
H	29.53349440688568	-22.95053707658318	4.53812130305280
H	30.89577955895353	-22.07196529452937	5.24351146407478
H	29.95591908528389	-23.18672705692386	6.23822084140199
H	30.66966876081961	-24.80922816645540	1.67647415913561
H	29.72158704679418	-25.99769466716121	2.57234858577283
H	29.42547406652929	-24.27107128705519	2.81007701465611
H	33.19827716878702	-27.89288573129261	0.05925735728663
H	33.89885454676318	-29.51156443411597	-0.05487244028202
H	32.41442016972802	-29.25065445171784	0.87026887010559
H	35.81403729705501	-30.35925972695799	0.51153050890233
H	37.26874228991666	-29.69863780430242	1.26898442393933
H	36.39214642145908	-31.01781036287556	2.04704630342930
H	34.02252734146675	-22.37137295580559	10.46042431872092
H	32.52614782045321	-22.85234154900792	9.65015454465115
H	33.63285539301531	-21.72741766591426	8.86015479266611
H	37.19039996663393	-23.95765908883568	10.40589417139942
H	36.22643572664616	-25.21682977340458	11.17919035258605
H	40.03689009382143	-28.94311671351652	8.47404774194680
H	39.66663767985438	-27.27069764096197	8.91259839568862
H	38.68277618674210	-28.58954401650882	9.55312091090918
H	38.87404438711133	-30.80173827927320	5.63009526287182
H	39.84595019027122	-29.52805902534147	4.88635505906470
H	40.13823301951426	-29.99553628939882	6.56665884995769
H	35.68934579276895	-23.53415387971057	11.23892641485498
H	31.76380457460583	-32.05437140587404	5.77047081675941
H	33.00270453046444	-33.32565878116100	5.75499115874259
H	32.98685166845136	-32.11700424653289	7.05414613055993
H	34.77550050564249	-31.54334646251116	5.42941801612782
H	33.59243824804952	-31.52580351060121	4.09996794862144
H	32.31167719966134	-26.60308537299989	7.52794439667099
H	31.73288494744620	-28.26587045952606	7.37953641775302

H	32.96294268099020	-27.86272673008820	8.57875180289511
H	32.02714785201137	-26.95461276797402	2.05973748734261
H	37.35969933928313	-26.35846858744075	9.29755260043691
H	37.56423788214622	-29.57010568922917	3.80291670466777
H	32.28300959433624	-23.15048700700683	7.16293316192797
S	36.03650237814390	-24.85530630744178	4.39668007632697
C	37.39814957837175	-24.27771306378736	5.47945199693477
H	37.01490145977224	-23.82112984263627	6.39881955978276
H	38.06581376711393	-25.10065564012658	5.75763905713300
H	37.98352195212732	-23.52552967313872	4.93774428654439

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B3LYP Scan/Thiolate IPC Model/Trip/290 degrees Constrained Optimization

C	30.19486476873507	-24.87413561821829	2.64367923784305
C	36.12651286668657	-24.40871343125117	10.61261649224768
C	39.24120480923111	-29.91106511829325	5.73888890931592
C	33.24817317353610	-28.77302549866179	0.60227119049808
N	33.07847682237239	-25.55194026945636	4.94999603723419
N	34.79889072680203	-25.40702304590746	7.24571316524984
N	34.70909069254926	-27.60697625743890	3.85728379924320
C	32.61811936365747	-26.78753072122207	2.89139061893280
C	32.91542654175210	-23.91600564292929	6.76646535357037
C	36.68512407782198	-26.47647719570886	8.377502228099228
C	36.78889467336416	-28.85708505669800	4.17276649405193
C	30.45286917180918	-22.88192908357923	5.20484780376051
C	33.63117113365108	-22.63991499966673	9.49795528432812
C	39.10918116405541	-28.38667613314031	8.61419915404751
C	36.11662621225833	-30.07694381284540	1.40483810869474
C	32.32926217195604	-25.81026379986197	3.83781756069168
C	33.97378015322094	-24.36284299687568	7.55383533825499
C	37.04962593248656	-27.36065236782300	7.36814002636977
C	35.65766315435455	-28.49789771030281	3.44805098191620
C	31.21619242290990	-24.87771977764710	3.74277641309760
C	34.32357206232430	-23.80412967312133	8.85236560515063
C	38.20039270755361	-28.24776160803371	7.42868953700965
C	35.29339038938084	-29.07527301395312	2.16036810951788
C	31.32538981598649	-24.03964182056698	4.81934725533463
C	35.37019174916792	-24.55032012158708	9.32445177729981
C	38.25294048036274	-28.89103772343940	6.22145150904489
C	34.08817018148468	-28.52568899608049	1.82020603885329
C	32.49321088785918	-24.48242428282133	5.56768876953378
C	35.65495965488419	-25.54547631626980	8.30214957382000
C	37.12086255007154	-28.40445018310003	5.44649498444410
C	33.74531525146632	-27.60172464148819	2.89222071249694
N	36.41677429324365	-27.47833514982210	6.16215836003077
Fe	34.74539651053343	-26.52516812474098	5.56232608641167
C	34.46727875259305	-31.36794314919950	5.63440423988808
C	33.41961393710393	-32.36675244334789	6.11102293569165
C	32.33204139456274	-27.56317079313773	7.26976149574691
C	33.61073202498383	-27.89449182328853	6.54814143534487
C	34.01692620458279	-29.28551777468236	6.72351587657662
O	34.43206695191017	-29.78833403359292	7.75688154280886
O	33.94265746195675	-30.03749313655428	5.56711064535661
H	29.61196010407358	-22.76426592980392	4.51281313266595
H	31.01086281428233	-21.93524606863949	5.20612792932847
H	30.03259324680600	-23.00582404713350	6.21241465600845
H	30.65109961771507	-24.67960358205993	1.66295697951640
H	29.67519433199175	-25.83926740852169	2.56687582482300
H	29.43172770174201	-24.10505483701624	2.80590265694000
H	33.05449752446034	-27.84580191612259	0.04555369342870
H	33.73735372854471	-29.47085771094936	-0.08605492188438
H	32.26897714046193	-29.19988760479300	0.86108337668307
H	35.65548519948310	-30.33147896851813	0.44406533570107
H	37.12570307389458	-29.69701298935814	1.19439966910322
H	36.24010052027110	-31.01387108598096	1.96611536327395
H	34.06970546953232	-22.40371939639697	10.47375705070910
H	32.56221470159186	-22.83871577714603	9.65792585839660
H	33.69721516391181	-21.73359102426062	8.88011403161426

H	37.17885153644015	-24.14140030525115	10.44107446138204
H	36.12671077662802	-25.34395475491264	11.18894181535560
H	39.92653987616754	-29.08815383875667	8.41475916148347
H	39.56288065032587	-27.42655145113434	8.89701509459554
H	38.56776980662099	-28.75662550379693	9.49579189878825
H	38.75833073733718	-30.87424656989307	5.52288253623945
H	39.73832130368017	-29.58826530964439	4.81379926136086
H	40.02302069966917	-30.09760311699414	6.48320856638768
H	35.69147483793186	-23.63180321544532	11.25083150245165
H	32.52473759283097	-32.31699038356435	5.48325473026401
H	33.81231069643724	-33.38995073038181	6.06921657899213
H	33.13457954203538	-32.14859548644440	7.14181390850234
H	35.33621469697403	-31.38168207578178	6.29557926980648
H	34.79011062885672	-31.59388700544976	4.61455444862824
H	32.14428084123094	-26.49184365989644	7.33136456107956
H	31.45648430586794	-28.01234383838445	6.76815101365655
H	32.33952590374084	-27.96213286833666	8.29675852858302
H	31.93461527965365	-26.88537293224579	2.05332912289963
H	37.28272911580442	-26.48405443691983	9.28389918637162
H	37.45247718978025	-29.58910122514666	3.72206264886857
H	32.34604744669124	-23.07060240815438	7.14068400572259
S	36.03453349066929	-24.90540719754678	4.37014141099936
C	37.36613283030364	-24.31816168016793	5.48506886899928
H	36.95874418938975	-23.84531211484057	6.38548188141328
H	38.01978803099539	-25.14085514389392	5.79551940209250
H	37.97254935995198	-23.57822805396033	4.94969175806641

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B3LYP Scan/Thiolate IPC Model/Trip/300 degrees Constrained Optimization

C	30.18415886628205	-24.84940762207627	2.65380905840057
C	36.11625146032948	-24.45712686737685	10.62356917476887
C	39.24579920327101	-29.89204923412693	5.68690247217396
C	33.18207262169496	-28.80014529447829	0.62166556586898
N	33.060933353825998	-25.56063511237803	4.95764259244632
N	34.78819986762724	-25.43092263682183	7.25030156581887
N	34.66530478238302	-27.63296204827750	3.86642540661751
C	32.56992472565307	-26.80984703900806	2.91428155263143
C	32.93427742481880	-23.90701967685068	6.76049264548930
C	36.65743587007481	-26.52679560342531	8.38286118500036
C	36.76656790741868	-28.85528034805060	4.14823849666158
C	30.49569346048542	-22.83162900751389	5.18907542106467
C	33.66874300751881	-22.63429837243745	9.49003686646222
C	39.10078201072109	-28.41733193968784	8.58741523676221
C	36.07294621856616	-30.07545053902027	1.38767409394602
C	32.30253393017539	-25.81686647951105	3.85164669476096
C	33.98229519541438	-24.37056251943792	7.55253710053259
C	37.01953568802418	-27.40439745836618	7.36636758070349
C	35.62091322813379	-28.50869675006260	3.44093337767100
C	31.20798010676312	-24.86313564146701	3.75048715137410
C	34.33984086951207	-23.81424029403334	8.85030415418350
C	38.18103235059758	-28.27834035109671	7.41009513447079
C	35.24838032484788	-29.08401755662973	2.15474587488355
C	31.34004820690619	-24.01414725690086	4.81621584498864
C	35.36866167730432	-24.58092283133652	9.32867092677151
C	38.23924898692012	-28.90059906029248	6.19128767556800
C	34.03262497131856	-28.54809707856902	1.83121509046896
C	32.50026138581026	-24.47309856651423	5.56610528499410
C	35.63808962518370	-25.58337173538733	8.30909024857568
C	37.09711010312331	-28.41938205840284	5.42805269041108
C	33.69301247023332	-27.63005233063747	2.90978769819040
N	36.38095238189433	-27.51729264381106	6.16204035674541
Fe	34.71327355736900	-26.55599365408741	5.57170390232566
C	34.72930465494972	-31.30670250345023	5.89579626132609
C	33.63633092972843	-32.35766463049023	6.04401250154122
C	32.20659954416117	-27.49715772357312	7.14457150402677
C	33.55102485882678	-27.88155774221535	6.58505662964880
C	33.89941322176347	-29.27047377599213	6.83664885240064
O	34.01184575711257	-29.78718309260890	7.94278809975667

O	34.18708042958704	-29.99824868824115	5.70095328537067
H	29.66174372410347	-22.69730346883190	4.49175611674968
H	31.07825538684599	-21.90000266764345	5.18609792883679
H	30.06716461819313	-22.93704468532312	6.19528350394086
H	30.64012425543527	-24.66188757581721	1.67154578745989
H	29.65307921270857	-25.80849253499700	2.58000958369709
H	29.43026171954174	-24.07146933580615	2.81676541067730
H	32.96878176845951	-27.87238878910838	0.07316632024614
H	33.67334137519941	-29.48661841504820	-0.07651440453398
H	32.21208284027276	-29.24277533737444	0.88867668280976
H	35.61284863209656	-30.31922283907924	0.42359682066547
H	37.08160206416369	-29.69180444114553	1.18249284113687
H	36.19670809357392	-31.01878768286562	1.93814906973363
H	34.14527759114339	-22.36901155747787	10.44023277710316
H	32.60770802393614	-22.83089673943916	9.69905863425976
H	33.70659923531762	-21.74667823520652	8.84381538313614
H	37.19396939779460	-24.31973246346930	10.45969011855871
H	36.00198036787538	-25.35423141130602	11.24806612482227
H	39.90765912300131	-29.13026439179789	8.38600961553930
H	39.56916625937826	-27.46000474847073	8.85581495853089
H	38.56545449939107	-28.77180838609043	9.47892797744207
H	38.77768018016325	-30.85220194900308	5.42944365136366
H	39.75159536450442	-29.53021700099317	4.78105419871841
H	40.01966482768432	-30.09603966410451	6.43491598255420
H	35.76254597342716	-23.60309929543003	11.21164671653028
H	32.94847811316553	-32.32092810654432	5.19376571887511
H	34.07026626838657	-33.36393540297262	6.09140614639507
H	33.06861355088214	-32.18189860997712	6.95959091483630
H	35.37941517023977	-31.30284533181774	6.77345400390600
H	35.33503371673736	-31.49378720562543	5.00510119617792
H	32.18042682566899	-26.47405645074137	7.52784905183907
H	31.42954144626980	-27.55111949632818	6.36501757005535
H	31.90312254511933	-28.16996762185665	7.95781698074015
H	31.87973572628693	-26.90644283851393	2.08153708041059
H	37.25628838132535	-26.54155423028834	9.28835684390801
H	37.44102255212746	-29.56610572908788	3.68000811698093
H	32.38162434186626	-23.04811612813312	7.12895413469060
S	36.01417528777444	-24.94255392707831	4.36805492386927
C	37.35689307249743	-24.36780086295099	5.47663881912765
H	36.95854325629021	-23.89687083842781	6.38211951023956
H	38.00832502243382	-25.19549554686936	5.77877522895485
H	37.96419976795246	-23.62871129231368	4.94106370321224

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C	30.18005752486200	-24.85829948938078	2.64278342333109
C	36.10117185367320	-24.48064873105868	10.62171286843455
C	39.24569317211795	-29.89147480424145	5.67396282185548
C	33.19826767104816	-28.78648045774244	0.59563573995196
N	33.05733191479724	-25.56850814301242	4.94544062097420
N	34.78024924983941	-25.44552371130839	7.24368381652789
N	34.66251084249672	-27.63782531666181	3.85593283735298
C	32.57008218291323	-26.81341468117905	2.89896764299704
C	32.92584704911332	-23.92195513009058	6.75437283297658
C	36.64191894023310	-26.54941502259373	8.38236865623943
C	36.77011606180037	-28.85020802231562	4.13416931346385
C	30.48640471820230	-22.84498488632757	5.18273857343140
C	33.65271778731705	-22.65648186473595	9.48795327115525
C	39.08545134678105	-28.44033833911140	8.58549451076324
C	36.09336266116886	-30.05168366083404	1.36273766725145
C	32.30012636865504	-25.82353780698989	3.83874319488999
C	33.97314726924321	-24.38575874296013	7.54596238827513
C	37.00665108333298	-27.42294068193955	7.36379874405417
C	35.62481973156235	-28.50416603367016	3.42645597030552
C	31.20355367557369	-24.87183755060549	3.73974962342424
C	34.32553381808633	-23.83472587588281	8.84696791333339
C	38.16972041773199	-28.29510798972501	7.40578589088908
C	35.26003433963101	-29.07135613954326	2.13458048715179

C	31.33321494260921	-24.02506643811947	4.80765812600310
C	35.35256098293242	-24.60347004580936	9.32711119733097
C	38.23419314200947	-28.90715985244856	6.18233419350015
C	34.04234802346659	-28.53996844856830	1.81085259478174
C	32.49458266660397	-24.48339819668046	5.55702249411675
C	35.62567717147353	-25.60229137987011	8.30546311725988
C	37.09316716612008	-28.42330793629171	5.41867280305617
C	33.69433727614836	-27.63148316962569	2.89493017268791
N	36.37105898839699	-27.52977898900209	6.15692521011845
Fe	34.70136219123281	-26.56994335597321	5.56746053799167
C	34.72972619750605	-31.30106825761145	5.91359746944112
C	33.59568927237981	-32.31972228895184	5.89278734840227
C	32.33994611496833	-27.41023229239150	7.37884830592922
C	33.53149508638350	-27.88330674487946	6.58417620824407
C	33.83501040366913	-29.27971821629418	6.81921134540130
O	33.78329080977558	-29.84338911293196	7.91081833579430
O	34.25623209525786	-29.97110564829928	5.70347797253438
H	29.64897082894167	-22.71463698406609	4.48886613911523
H	31.06575776612214	-21.91135021566160	5.17604931449843
H	30.06270626608873	-22.95069723143497	6.19088440227504
H	30.63687605460563	-24.67323219180809	1.66048797534736
H	29.64765841485542	-25.81676143797880	2.57048082009796
H	29.42735776714834	-24.07886527252012	2.80401257811147
H	32.98975311775618	-27.85654879388533	0.04891938676113
H	33.69245787692515	-29.47142395190211	-0.10197138859950
H	32.22607871151433	-29.22833390125896	0.85559903695643
H	35.63552562444713	-30.29502100985214	0.39749197687226
H	37.09857710046638	-29.65810679129398	1.15932783206124
H	36.22549444158140	-30.99626308596850	1.9089900283101
H	34.10603870701365	-22.41358311507049	10.45528516043710
H	32.58402333181121	-22.84286789441994	9.66384831679219
H	33.71988938677465	-21.75849519164194	8.85844819315339
H	37.17034713717432	-24.28698866505717	10.45697879776698
H	36.03405092853107	-25.39983347449948	11.21992105367692
H	39.89755618777870	-29.14619262217376	8.38025304422337
H	39.54665483083023	-27.48292842421937	8.86564859425768
H	38.54878637933591	-28.80710870235464	9.47132216606937
H	38.78278179833359	-30.85334932197078	5.41348779134480
H	39.74881817348717	-29.52366042636147	4.76908374970503
H	40.02123681375041	-30.09373109846626	6.42072754326336
H	35.71046319759775	-23.66196058336612	11.23589280617758
H	33.01973822559407	-32.23508955476437	4.96636967777479
H	33.99062253160756	-33.34080526213334	5.96118899324711
H	32.92552494584230	-32.15031589532352	6.73732176853613
H	35.27011643188021	-31.35205405228541	6.86172354129933
H	35.43034721583052	-31.48054258179297	5.09347360262436
H	31.70148846276874	-26.75304740942159	6.78227087292709
H	31.73370686358469	-28.24314446355257	7.75370072253684
H	32.64471974159567	-26.82140194040554	8.25632600796357
H	31.88190080702644	-26.90843656762839	2.06442483745599
H	37.23697460836397	-26.56766107957833	9.29029152238479
H	37.45024419859627	-29.55313047139910	3.66219830107273
H	32.37111359540922	-23.06548295103935	7.12533689071588
S	36.00270866587017	-24.94745117546517	4.37461791133692
C	37.35412333510025	-24.39179708939913	5.48210318003800
H	36.96241209002637	-23.92935663853110	6.39488018373024
H	38.00379864385970	-25.22540168692280	5.77154262594288
H	37.96142158305760	-23.64913433746717	4.95155582559439

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C	30.17153938428554	-24.83297249352619	2.67134535060480
C	36.10240679327802	-24.52751011206905	10.64149079215138
C	39.26453915684360	-29.86123500291967	5.62382013653413
C	33.14200261295931	-28.79683030064905	0.61863955959270
N	33.05207893011610	-25.56969642214914	4.96131504398363
N	34.77921617403896	-25.46812657753930	7.25734966642024
N	34.63359435526067	-27.65558813359965	3.86872183726645

C	32.53609349185233	-26.82347927674939	2.92775698448614
C	32.95444518714118	-23.91075021038084	6.76066981683336
C	36.63199298021210	-26.59024275202210	8.38970712436042
C	36.75716814698109	-28.84545455982286	4.11638377897046
C	30.52618743428639	-22.80528987381368	5.19322692359899
C	33.69812479044288	-22.65542145419960	9.49555410432360
C	39.09391944165650	-28.46088869589656	8.55817216796831
C	36.05230881410777	-30.04923118095833	1.34968440204166
C	32.28418300751246	-25.82288031342972	3.86192333503908
C	33.99191355423831	-24.39212852976048	7.55571159919771
C	36.99790653647117	-27.45027553488528	7.35932873651875
C	35.59761745775977	-28.51328392863708	3.42535065586445
C	31.20119763917481	-24.85536536162351	3.76241246866382
C	34.35167572399204	-23.84576794081704	8.85693478420372
C	38.17040837200998	-28.31095085048329	7.38503109835286
C	35.22123568885260	-29.07816693708772	2.13562496896526
C	31.35172000920382	-24.00168784522615	4.82222345710860
C	35.36198914150665	-24.63356594743704	9.34092498634260
C	38.23916656447897	-28.90119833413027	6.15105162096766
C	33.99669332992715	-28.55255175433121	1.82696008288092
C	32.50975061604735	-24.47238643901526	5.56814648958149
C	35.62121954970174	-25.63682460091404	8.31970377881435
C	37.08835203078201	-28.42123463499892	5.39953735959835
C	33.65635106465606	-27.64769026403273	2.91629629247656
N	36.36060872980727	-27.54594810721744	6.15320782730293
Fe	34.68688718045799	-26.59157509551813	5.57957895081884
C	34.87101172173993	-31.27999980629588	6.19086531325302
C	33.78215209377115	-32.27585367759897	5.80532423144864
C	32.20244414114870	-27.40240359099917	7.19775404415055
C	33.48720284606479	-27.88842286327857	6.57823999510635
C	33.74411207544595	-29.28517476507264	6.86488238334943
O	33.38663238331402	-29.89342451351959	7.87567261603115
O	34.48879417890393	-29.93643932709478	5.90537999807076
H	29.68949786609857	-22.66392726694444	4.50069738935923
H	31.12154731795721	-21.88188530579459	5.18030960626510
H	30.10332426326805	-22.89873918970857	6.20294789522185
H	30.62358801961399	-24.64812942564548	1.68673197049976
H	29.63274308834045	-25.78782147922856	2.59990753726178
H	29.42461440212252	-24.04937956438758	2.83915263244925
H	32.93574283367763	-27.86694974160648	0.07085920113637
H	33.62615852059457	-29.48711402856140	-0.08068683943716
H	32.16869842159616	-29.23109644485731	0.88693118929903
H	35.58414568710106	-30.29276142467403	0.38944580079730
H	37.05144851876296	-29.64639360998155	1.13485904393258
H	36.19911817351154	-30.99428990403378	1.89109526052194
H	34.17174933006297	-22.40274902346562	10.45060254312506
H	32.63194121172404	-22.83276268604375	9.69510478095953
H	33.75820878465129	-21.76637482058115	8.85301782584577
H	37.18372224115369	-24.41018087118019	10.48590705978764
H	35.96635951780835	-25.42391311016248	11.26266421658583
H	39.90382226451641	-29.16703449239602	8.34533154412817
H	39.55823434248673	-27.50491364155818	8.83834522135420
H	38.56339259038162	-28.82964495124724	9.44688664510684
H	38.81771047953283	-30.82677730746167	5.34890746671041
H	39.75875660857582	-29.47055906280607	4.72365322727021
H	40.04559482635252	-30.06261026940786	6.36503113389265
H	35.76098983657832	-23.66851151205170	11.22959136300691
H	33.49322025740726	-32.13963030740509	4.75897323949915
H	34.13391610126808	-33.30662163596098	5.93551206905520
H	32.90145751357228	-32.12838016480593	6.43259979092766
H	35.11622736768474	-31.37536890533351	7.25133134520306
H	35.77532529641659	-31.44335644363056	5.59792200244809
H	31.45434245112493	-27.20391551566187	6.41739965438760
H	31.78678562401065	-28.14080570314362	7.89033432986471
H	32.32668930289202	-26.45878457945892	7.73668611322041
H	31.84096155289388	-26.91673889444967	2.09873175486361
H	37.22858923980534	-26.61758080792777	9.29641839073409
H	37.44111414528993	-29.53653913743817	3.63252524258586

H	32.41618706325995	-23.04214284025711	7.12765374110636
S	35.99302147669818	-24.96767406557469	4.38379044943274
C	37.34834531117502	-24.41436641425025	5.48794041197133
H	36.96031649886747	-23.95183905220851	6.40231849058255
H	37.99782846127064	-25.24897496200220	5.77509489625558
H	37.95520485946240	-23.67212042700578	4.95628659953775

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C	30.15584202576496	-24.89854217968772	2.67133599642934
C	36.11206842921913	-24.45323666147962	10.61839998347994
C	39.27388025354823	-29.85026989869067	5.67193938652806
C	33.16723043210281	-28.83644314992126	0.64180763292945
N	33.03720917735629	-25.59991319342666	4.97191944295226
N	34.77337176402798	-25.45602393960876	7.25851555908293
N	34.64233546815070	-27.66992465548924	3.89051539797962
C	32.53399680634351	-26.86918473277904	2.94581962955136
C	32.93640227653652	-23.91685516919760	6.74881278811948
C	36.63225748976965	-26.55762843526461	8.40286468532408
C	36.77511755609205	-28.84180385759203	4.14620714240602
C	30.50318047545284	-22.83875845649007	5.16853107968608
C	33.69054557250281	-22.61326954723179	9.45670001090416
C	39.09589673156120	-28.42574671207367	8.59428920282554
C	36.09394695721886	-30.04923692821965	1.37619607411294
C	32.27192907233564	-25.86605767273432	3.87396632367574
C	33.98071957970831	-24.38055342953882	7.54450234300963
C	36.99935714287481	-27.43010336596660	7.38379283860854
C	35.61670651090773	-28.51724404127287	3.44984090508246
C	31.18499095128961	-24.90418254138142	3.76301306200065
C	34.34447948091245	-23.81214865605566	8.83435008913922
C	38.17394415021895	-28.28740125315980	7.41850723650994
C	35.24936254170484	-29.08844043239256	2.16044443069153
C	31.33168434279861	-24.03762288795574	4.81246763231052
C	35.36185461621292	-24.58709066694408	9.32585515453994
C	38.24642249662703	-28.88732005329450	6.18954718402105
C	34.01779550006668	-28.58030876291949	1.85066103964742
C	32.49116754430008	-24.49594389288358	5.56489845591878
C	35.62079264237592	-25.60511752257266	8.31966983003412
C	37.09597976666316	-28.41613342560956	5.43175271299053
C	33.66505774158573	-27.67811055231306	2.93832683639887
N	36.36285106924360	-27.53892222465625	6.17777967440022
Fe	34.68285151332761	-26.60162667665649	5.59921014918420
C	34.75460899911412	-31.31322128777511	5.98243332739540
C	33.61986366872414	-32.23730281670341	5.55128600548375
C	32.39905991011624	-27.38568993849098	7.49339085617031
C	33.51894227438449	-27.90095537682505	6.62460892649992
C	33.72826206287088	-29.32256397494465	6.81039534564910
O	33.35813577200460	-29.98116094751743	7.78442781048987
O	34.42571934018291	-29.93922134680204	5.79429643353657
H	29.67344285643579	-22.70077890567136	4.46695381363742
H	31.09981007740705	-21.91623949826971	5.15541897021164
H	30.07034142090907	-22.92488512221809	6.17474820339689
H	30.60666347667103	-24.71799435798676	1.68536379669552
H	29.62474944259323	-25.85823032012243	2.60760640760371
H	29.40253252969631	-24.11969621233469	2.83269910787993
H	32.97499526132202	-27.91467007765175	0.07520723714427
H	33.64684448279981	-29.54567425477104	-0.04150793467939
H	32.18755139510861	-29.25399016961644	0.91275991544037
H	35.63114972058156	-30.29734071115931	0.41453766308621
H	37.08867072403969	-29.63435037841448	1.16403481376248
H	36.25082570204130	-30.99308984820189	1.91698362160325
H	34.17528039314917	-22.33702714959401	10.39959839807344
H	32.62843297411766	-22.79349536942635	9.67457507114720
H	33.73576525201555	-21.73797904624636	8.79455708970846
H	37.19158677599309	-24.33530376262884	10.45145844915553
H	35.98462831938602	-25.33745561437653	11.25867853753885
H	39.89477238340640	-29.14857409905190	8.39622422574241
H	39.57528458457316	-27.47122554198406	8.85367467965839

H	38.56051510885302	-28.76740046024462	9.49078076873767
H	38.82538928875650	-30.81262331788486	5.38907621360564
H	39.78064061159031	-29.45941631553870	4.77871890807750
H	40.04538901207069	-30.05719338120749	6.42160864983751
H	35.77219719273798	-23.58392631912035	11.19200533405637
H	33.32135545931028	-32.02095205009007	4.52098916525299
H	33.93264175230441	-33.28745931092565	5.60566202452024
H	32.75475199057330	-32.09915140053587	6.20172183820368
H	35.01162558646750	-31.49088377888239	7.02989749469809
H	35.64250283804819	-31.47214348993944	5.36398022356628
H	31.85284118841770	-26.57328500597226	7.01167062085486
H	31.69568834407134	-28.17861745151253	7.76905138529431
H	32.78975840779131	-26.97857623124562	8.43821043500822
H	31.84127625985594	-26.97383040192222	2.11624017174051
H	37.23063617516245	-26.57012947783521	9.30878278227178
H	37.46580094429009	-29.52887232624602	3.66625426098316
H	32.39340552629223	-23.04762733847356	7.10711879123509
S	35.97160344652497	-24.96577853421751	4.38823820273224
C	37.34089484836623	-24.41478273221130	5.47602511916468
H	36.96384482903537	-23.94983360044694	6.39380895560003
H	37.99149105770722	-25.25063960046695	5.75706683429378
H	37.94408725332785	-23.67487277083667	4.93695813775934

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B3LYP Scan/Thiolate IPC Model/Trip/350 degrees Constrained Optimization

C	30.12422519667259	-24.97617335698239	2.72708819356353
C	36.14251773879703	-24.41376685973442	10.61579646814137
C	39.30074497847981	-29.83571263712446	5.70007225026981
C	33.15877370085826	-28.90082185091425	0.69894533991797
N	33.04887572393475	-25.61444346878492	4.99021923344313
N	34.79192576252286	-25.44862935829288	7.27093408443513
N	34.65091066859981	-27.69145262059430	3.92389044877024
C	32.52741119818486	-26.91811679366213	2.99107126865281
C	32.95531295841208	-23.91301618967941	6.74974981969684
C	36.65175423213213	-26.54191788226342	8.42142818121217
C	36.79287434212501	-28.84682725443227	4.17687433584670
C	30.49299122367010	-22.87376067161164	5.18569895063266
C	33.71895891249822	-22.58211345949260	9.44278546264165
C	39.12208648082798	-28.40076831293807	8.61745028438598
C	36.10736812813138	-30.07447276125646	1.41626781676643
C	32.26967160842966	-25.90364018045693	3.90812245549980
C	34.00221922438627	-24.36831785740511	7.54713929958946
C	37.01747776709723	-27.42081622083977	7.40740549696590
C	35.62947361862809	-28.53390203330659	3.48336571965260
C	31.17248222039538	-24.95308244893992	3.80014677557769
C	34.36915839995986	-23.78846628129828	8.83103942273651
C	38.19619622430898	-28.27304558112284	7.44352783061523
C	35.25647791745878	-29.12061201982606	2.20261838133505
C	31.32809144315126	-24.06919867562323	4.83376371056727
C	35.38541780922114	-24.56120993805320	9.32862519662476
C	38.26905226396273	-28.87689347087365	6.21678695917157
C	34.01629436361722	-28.62802440685492	1.89942368706120
C	32.50265237951584	-24.50691461172161	5.57571756858004
C	35.64045492576201	-25.58960676629381	8.33198743566393
C	37.11473359995500	-28.41362352866087	5.45940490595915
C	33.66525314615377	-27.71771659551648	2.98073189387726
N	36.37863716597537	-27.53795900219670	6.20393639558067
Fe	34.69425916830553	-26.60929923453150	5.62284487942692
C	34.67111846084986	-31.31685656751077	5.96492819249122
C	33.60300678956281	-32.09187186465501	5.20035189609760
C	32.40524546534445	-27.34591270625606	7.52475455423340
C	33.50908491313908	-27.88768590376206	6.65301382363057
C	33.62821539465237	-29.32721907379550	6.77380164513559
O	33.05796573147780	-30.03493476256944	7.60872641649372
O	34.48015301909972	-29.90953083907731	5.86053407294054
H	29.64766211605199	-22.75779141879866	4.49888980732935
H	31.07802015224280	-21.94456099806619	5.14510785436562
H	30.08154963722284	-22.94811369239383	6.20171869322422

H	30.55765100934745	-24.82394787008270	1.72867610142808
H	29.59144871226132	-25.93669214821114	2.69987428835303
H	29.37458460210548	-24.19211796481474	2.87996649025264
H	32.96362258493713	-27.98684527326049	0.12077938607803
H	33.63443439189187	-29.61958346471045	0.02288096720616
H	32.18068035789479	-29.31427818761549	0.98127626556947
H	35.62648326519172	-30.35666402935767	0.47312587821257
H	37.08365479994767	-29.63590385415904	1.16862257036580
H	36.30618260082053	-31.00081378231003	1.97285163216449
H	34.19176234626399	-22.31102760409878	10.39317949526048
H	32.65177047849094	-22.75116807418656	9.64371187441714
H	33.78382718013363	-21.70717715333552	8.78163258784309
H	37.21597270366074	-24.25680150810608	10.44070331631233
H	36.05190462447030	-25.30803035680821	11.24806377729812
H	39.93243023286890	-29.10965357302085	8.41566600376013
H	39.58595898042006	-27.43941410122867	8.87959056437974
H	38.59415867529496	-28.75415669652653	9.51397487635252
H	38.85745626981552	-30.80247521754166	5.42399553300985
H	39.80123415132191	-29.44633258272498	4.80271456969923
H	40.07659929288787	-30.03387743813522	6.44765197036566
H	35.77813974293120	-23.56243545369733	11.20111106861710
H	33.55813273993252	-31.75395192121945	4.16124782198214
H	33.82293217357778	-33.16654391608525	5.20633982681951
H	32.62537281055536	-31.93636528398791	5.66013054052735
H	34.67497274119241	-31.61082408907165	7.01734850045022
H	35.66179626788343	-31.49766602468793	5.53781207604322
H	31.85227851725605	-26.54387110369030	7.03215275962920
H	31.70793090070726	-28.13112168181969	7.83045266236239
H	32.81517993017391	-26.90835070426130	8.44679811428642
H	31.82432958838258	-27.04115969414926	2.17282841962900
H	37.25205134985583	-26.54706964357072	9.32619982590234
H	37.48613812446740	-29.53208988509207	3.69805317318615
H	32.41414954699268	-23.03943789504023	7.10031862839233
S	35.98066091412635	-24.98117703601230	4.39618188296808
C	37.36049527442474	-24.43195491539561	5.47141799446331
H	36.99200115386083	-23.96176158223775	6.39003537972992
H	38.00964795068494	-25.26921691733896	5.75148979304401
H	37.96270184119285	-23.69651821423814	4.92517327483557

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B3LYP Scan/Thiolate IPC Model/BSS/0 degrees Constrained Optimization

C	30.71368473158898	-24.78756069722472	2.33608666514346
C	35.86445107795909	-24.56680450853815	10.83129328895996
C	39.24471283818192	-30.13239546688735	6.26832600470909
C	33.74780078987580	-28.82103209399733	0.61157764394867
N	33.29863416106671	-25.57923762503444	4.94038992985082
N	34.75359735733827	-25.53037709512299	7.37833944623356
N	34.91563188502459	-27.78009890877522	4.02346204714104
C	32.98706752562387	-26.82603693772490	2.85504205117204
C	33.02414016609858	-23.92650945439178	6.72417242049421
C	36.47962244052128	-26.69142229087767	8.67188570638994
C	36.93298188805706	-29.07483419271594	4.49839896115179
C	30.78502471285957	-22.79126009374194	4.90564263679872
C	33.59048670904945	-22.65609696704326	9.49807519298989
C	38.86760393101285	-28.60914885161710	9.11858603433495
C	36.48755689560448	-30.23262064729398	1.65651405599098
C	32.66032795361473	-25.81646913454471	3.75617064469432
C	33.97615141137108	-24.42794426398091	7.60776334145265
C	36.90122372920465	-27.60078239970530	7.70735148620318
C	35.87423923028894	-28.68895752307581	3.68332802515002
C	31.60989193047505	-24.83152456249654	3.53872821605119
C	34.25352443745712	-23.87421534432756	8.92497439955086
C	38.04607018650152	-28.48861387949721	7.86901253127116
C	35.61943115140134	-29.22660265391218	2.35447930958726
C	31.64130581039672	-23.98908323861046	4.61777687197507
C	35.20764951008295	-24.67971038116630	9.48706751159943
C	38.20381323052035	-29.13033399043772	6.67160602104719
C	34.47023157118786	-28.62830261899866	1.91199837379159

C	32.69927247842262	-24.47946845283106	5.48859993475040
C	35.51200901973327	-25.70597293051080	8.50049535031975
C	37.13799539239429	-28.64712285453918	5.80492289124311
C	34.05909647078952	-27.70697100744760	2.96386072747214
N	36.36594475056194	-27.73192447769312	6.45928115651834
Fe	34.78960491478145	-26.69788109106653	5.72625837334633
C	34.49498659390609	-31.41125453854822	6.00890627173741
C	33.70652448717331	-31.99899946924596	4.84441246826268
C	32.17731212489829	-27.33101021795265	7.12405270388365
C	33.43034328511509	-27.90110405429522	6.51203730458593
C	33.38575353938649	-29.37282849946687	6.53954694876060
O	32.46580961873646	-30.05039125551206	6.99308347968249
O	34.48055953997474	-29.98357937855970	6.00152073896826
H	30.04540729395304	-22.62440306270084	4.11476047301982
H	31.38307361958066	-21.87355132838017	4.99366053146306
H	30.23349288061014	-22.90282198333288	5.84959031184873
H	31.28526738016080	-24.65289501268726	1.40735596873787
H	30.13731649386957	-25.71640014522144	2.22281869698485
H	29.99512476309256	-23.96315623402226	2.39976633252426
H	33.65724711663385	-27.87961224818564	0.05234995874816
H	34.26923483174463	-29.53542169632207	-0.03477524880107
H	32.72762610798336	-29.20054249346068	0.76381222836108
H	36.11106003477136	-30.46025274652633	0.65321334636190
H	37.51818263894946	-29.86861604281504	1.54480449246332
H	36.54320552449711	-31.18152478871314	2.20809353196648
H	33.97611159806408	-22.42243532734678	10.49649968989071
H	32.50301054462711	-22.78689894951037	9.58947071521590
H	33.75249720961848	-21.77090722443637	8.86745117002205
H	36.95145952906509	-24.43358304743754	10.74198914974203
H	35.70420595724447	-25.46704001616557	11.44088314605464
H	39.67777258411252	-29.33637999278536	8.99704005546668
H	39.32674048521130	-27.65095311825622	9.39931043942769
H	38.26156372347662	-28.93524106411066	9.97572760281341
H	38.79793465276429	-31.09179751045469	5.97188407373691
H	39.83627189480945	-29.77903250576777	5.41236303775003
H	39.94475367167050	-30.33839638709505	7.08572326635142
H	35.47509407470621	-23.71472354989227	11.39908289603269
H	34.05860168713476	-31.58287265150445	3.89699493088873
H	33.82617361892337	-33.08876588988805	4.81310455125395
H	32.64520697186350	-31.77043402091113	4.95222132332805
H	34.10337546463929	-31.77666150241108	6.96181064934684
H	35.55366708901770	-31.67170824833244	5.93296984060726
H	32.35700544132288	-26.38077805282468	7.62345623664903
H	31.43846917581345	-27.12721080948690	6.33392423086043
H	31.70468541910064	-28.02847879311629	7.82077114057830
H	32.39011680099692	-26.88800650825801	1.95000662097357
H	37.00338912322131	-26.70503700947973	9.62311132155638
H	37.63820152507184	-29.79441849334833	4.09313276037835
H	32.47056380422276	-23.04620643481649	7.03651736214755
S	36.46663358264546	-25.23440659981630	4.70404668240498
C	36.02788038206576	-23.47664694814991	4.98328703611091
H	35.05303546196515	-23.22732604538661	4.54892171698991
H	35.99750761796592	-23.23059946636639	6.05115145866567
H	36.78724942957341	-22.84465210086759	4.50738350986315

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B3LYP Scan/Thiolate IPC Model/BSS/10 degrees Constrained Optimization

C	30.70259018414226	-24.79572671324000	2.34106149116163
C	35.87770674109503	-24.55118411648581	10.82145581885843
C	39.22663042017177	-30.15027495762645	6.27434318102283
C	33.73582044251324	-28.82529374852399	0.61495790781453
N	33.28715342931581	-25.58729168046913	4.94574449564036
N	34.75573380095091	-25.52561597554963	7.37514644835394
N	34.89869783265590	-27.79560399537274	4.03198989447656
C	32.97282549172595	-26.83653101165434	2.86220091361677
C	33.02068534027204	-23.92693993996574	6.72371271066543
C	36.48435679747128	-26.68400513966385	8.66767821849788
C	36.91858744680366	-29.08742528955199	4.50404098808338

C	30.77960918814501	-22.79394728240359	4.90607447557654
C	33.59842777693301	-22.64527030117503	9.49004289992418
C	38.86141140783950	-28.61424592726459	9.11935675891452
C	36.47479065408240	-30.23843725245417	1.65684902901111
C	32.64731747691923	-25.82612240359322	3.76258399988379
C	33.97796437343028	-24.42335763788816	7.60419721748893
C	36.90059008426105	-27.59834775920571	7.70568031261729
C	35.85796679960467	-28.70348928240768	3.69011444414515
C	31.59860686626349	-24.83964734678481	3.54383464290346
C	34.26002984326633	-23.86491032099247	8.91844627372422
C	38.04063462714940	-28.49214545869210	7.86948389250105
C	35.60493636261952	-29.23669640568001	2.35900369183510
C	31.63227323704560	-23.99503461538141	4.62106182257083
C	35.21667445716764	-24.66812364742820	9.47963886420661
C	38.19341873902574	-29.13905062194466	6.67439113925197
C	34.45634801113471	-28.63672260018371	1.91698702649329
C	32.69040931488011	-24.48508733202888	5.49195343099205
C	35.51786926186228	-25.69750877876241	8.49528642594101
C	37.12928615439394	-28.65293590560865	5.80716905917092
C	34.04374224651466	-27.71885052265557	2.97081985816915
N	36.36332398996093	-27.73103596908418	6.45888279448135
Fe	34.78237003679367	-26.70205200853439	5.72944950693526
C	34.48052847707674	-31.41967471597727	6.05941435220587
C	33.82683566259248	-31.93755027479337	4.78358871135023
C	32.19259425366274	-27.33241910540882	7.17374677518265
C	33.42891489344400	-27.90154989063467	6.52733235954113
C	33.35253163004403	-29.37043705840759	6.49257119029356
O	32.35476245290923	-30.03501868329307	6.76333078124646
C	34.50700612338890	-29.99231429426495	6.11733337483334
H	30.03956252401955	-22.62762456718682	4.11548783880810
H	31.38038371133043	-21.87764500149777	4.99021314105168
H	30.22889880632877	-22.90068814218915	5.85104812767150
H	31.27465309707984	-24.66244482946186	1.41240113491282
H	30.12523409331888	-25.72398278445374	2.22847901921567
H	29.98506163183230	-23.97035439372064	2.40378611701362
H	33.64597821964838	-27.88210169394700	0.05865786826530
H	34.25808208231417	-29.53766773775923	-0.03291687154568
H	32.71557539664861	-29.20544127736517	0.76496061278823
H	36.10365105664776	-30.45519879877947	0.64917721201020
H	37.50685191142139	-29.87581883757525	1.55494037699602
H	36.52466088134577	-31.19331357262220	2.19872899273389
H	33.98649277194044	-22.40907312645906	10.48692688444835
H	32.51117704213480	-22.77576727482112	9.58439559777956
H	33.75895257125135	-21.76171334894573	8.85675076125020
H	36.96435456003216	-24.41750983125270	10.72859161029513
H	35.71994782240765	-25.44998843856860	11.43383782825705
H	39.66563182994199	-29.34854369393903	9.00073931225193
H	39.32838211045364	-27.65877212782798	9.39651212972961
H	38.25269927068241	-28.93207005611343	9.9772093281691
H	38.77212417662243	-31.10674713541527	5.98023372361592
H	39.82165393010493	-29.80433652637897	5.41770859706593
H	39.92448017309110	-30.35971361462256	7.09274251731305
H	35.48944134901314	-23.69796277572553	11.38829125701167
H	34.29717684658701	-31.49167778904776	3.90400795346423
H	33.92731756151190	-33.02789554203932	4.71957397047598
H	32.76573462423041	-31.68590658739807	4.77477617426439
H	33.96407228625534	-31.81156370006216	6.94008440107681
H	35.53321035755040	-31.70959887021819	6.10333525704823
H	32.39408762788010	-26.39670513954641	7.69227480726847
H	31.44196848109305	-27.10175458089410	6.40282241754394
H	31.71972666076854	-28.03895490882311	7.86212274078054
H	32.37633669961036	-26.89745504140427	1.95681260307138
H	37.01018745321176	-26.69561852758653	9.61780341145400
H	37.62123733131245	-29.81003947015621	4.09973578488756
H	32.46831643762210	-23.04537720886935	7.03466888671777
S	36.45379902658783	-25.24499866987095	4.68975423431825
C	36.03121330928966	-23.48624263559043	4.98619894237024
H	35.05151423877664	-23.22838557777714	4.56791444496966

H 36.01826774680199 -23.24644856113387 6.05581214373933
H 36.78742664676871 -22.85630173191698 4.50264433120961

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B3LYP Scan/Thiolate IPC Model/BSS/20 degrees Constrained Optimization

C 30.67804586045330 -24.82907838492289 2.35996330570452
C 35.92255684283490 -24.50347133312264 10.79699882535184
C 39.20997033589305 -30.17333483805729 6.29460712998276
C 33.76387067453255 -28.80297488887305 0.60360333747477
N 33.27991920336203 -25.59831440721505 4.95400290817028
N 34.76200434820385 -25.51945329558191 7.37510269716974
N 34.89226942572162 -27.80946118300158 4.04299578574346
C 32.97311955240129 -26.84418873324091 2.86699081373397
C 33.01209082759409 -23.93499029012784 6.72917635336904
C 36.50332759967723 -26.66338388298244 8.66365244411661
C 36.90488594544144 -29.10990758114558 4.52252473445277
C 30.74476354982142 -22.82993371756177 4.92718373065520
C 33.61720657980563 -22.62228311364317 9.47448067962423
C 38.87522218021114 -28.59763293575728 9.12161638571689
C 36.49138543999914 -30.22758603478116 1.65746011103016
C 32.63897087801811 -25.84100178076648 3.77209962111238
C 33.98223651758173 -24.41811788570917 7.60257667119146
C 36.90716423458085 -27.59199226443405 7.71035435234560
C 35.85291677811875 -28.71658970470801 3.70197789857129
C 31.58001213430849 -24.86459181406330 3.55853662961201
C 34.27725618396380 -23.84511246807132 8.90773317160040
C 38.04393814362292 -28.48927974609482 7.87734210529648
C 35.61322197302380 -29.23538868229982 2.36274631729197
C 31.60913056724173 -24.02130936787637 4.63689156782939
C 35.24416320996094 -24.63836932574759 9.46551443162122
C 38.18406965811280 -29.15291750620596 6.68996492652701
C 34.47020038369497 -28.62938142076682 1.91525731712101
C 32.67578357461915 -24.50155629836412 5.50289550868450
C 35.53666616481939 -25.67751137188340 8.48862049482743
C 37.11735847040642 -28.67092730386528 5.82372530964770
C 34.04707108184108 -27.72276295949793 2.97441685044745
N 36.36009664070899 -27.73767333454937 6.46912267225960
Fe 34.77862162226074 -26.70833646254956 5.73684158156887
C 34.37057934745361 -31.45235768256275 6.08420607396169
C 33.89563666814379 -31.91341444357752 4.71178486538221
C 32.21743657059734 -27.33387748736311 7.23648316672892
C 33.42649910645216 -27.90043499887037 6.53600060872286
C 33.29029779785625 -29.35796078534393 6.39937686744839
O 32.22845688553048 -29.97087829700893 6.46633342753140
O 34.45968203016459 -30.02851778731477 6.18784409425850
H 30.00097476876848 -22.66952802176289 4.13889479118253
H 31.33599460064994 -21.90752095358863 5.01214918957029
H 30.19758595016797 -22.94492755990493 5.87326414971031
H 31.24468775733904 -24.69320549414283 1.42836969518894
H 30.10699750028069 -25.76172347703037 2.25191292247095
H 29.95492811177350 -24.00876813757912 2.42485797818896
H 33.67546661771897 -27.85240868856813 0.05994779252565
H 34.29603130823820 -29.50375512139213 -0.04884161951783
H 32.74401038731965 -29.19004088427764 0.73797668208590
H 36.13692923990847 -30.42409793059801 0.63972716461440
H 37.52603239035032 -29.86643124259722 1.58042098383140
H 36.52913573060086 -31.19322065768193 2.18126616944999
H 34.01690304747910 -22.37336658780356 10.46367110715820
H 32.53186923621270 -22.75680723974861 9.58424501074314
H 33.76523137267341 -21.74491558309156 8.82968048077824
H 37.00724900561340 -24.36614687795132 10.68793381985320
H 35.77725962691529 -25.39571569894694 11.42198417601675
H 39.67610743899440 -29.33597190798991 9.00544458211643
H 39.34764934609321 -27.64002692527133 9.38169337488088
H 38.27354600925926 -28.90195800667763 9.98976013967721
H 38.74869559429771 -31.12937086187772 6.01007726745400
H 39.80367388938438 -29.83785713641112 5.43282958096078
H 39.91000585917910 -30.37970512505948 7.11195148546358

H	35.53816306359398	-23.64542601543880	11.35920564034730
H	34.52551715678645	-31.49241131250422	3.92540809391311
H	33.93441730219221	-33.00749722788848	4.64433912833607
H	32.86846086511294	-31.58956494975772	4.54278984462987
H	33.70412467284952	-31.83145673440302	6.86429291885000
H	35.38723145035838	-31.80043062139705	6.28348190619801
H	32.45487331688496	-26.42794443983223	7.79157227448813
H	31.45271745951532	-27.05567697617265	6.49658218198199
H	31.74353295431123	-28.05810013159534	7.90711390971817
H	32.37963330225998	-26.90316113392796	1.95955782719966
H	37.03824174095245	-26.66412492054232	9.60878925469900
H	37.60406536798852	-29.83787411883866	4.12185688481796
H	32.45563805772832	-23.05609341402501	7.04042135077998
S	36.44400914037984	-25.25954736012544	4.67999673971288
C	36.03699943320319	-23.50044165221313	4.99668218978479
H	35.05386736252130	-23.23258097232978	4.59314380732659
H	36.03960483787247	-23.26979880964856	6.06832346082536
H	36.79131942223439	-22.87142338989749	4.50893429410099

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B3LYP Scan/Thiolate IPC Model/BSS/30 degrees Constrained Optimization

C	30.68225964313374	-24.86533204130089	2.33158518230575
C	35.91753894887170	-24.45970364585272	10.77410037630761
C	39.19963522861896	-30.18280352093140	6.33633946210904
C	33.81943366224951	-28.79876625587733	0.58607732607433
N	33.26431394217675	-25.62475548039601	4.94801442341782
N	34.74387762282920	-25.52184647939471	7.37014105127014
N	34.89947412394974	-27.82293756416949	4.04632991368356
C	32.98527853245847	-26.86614967853546	2.85517345929902
C	32.98672175811353	-23.95176676336700	6.71354633697372
C	36.49250327412658	-26.64679225681143	8.66641621756715
C	36.91265181946352	-29.11713072252149	4.54164362981833
C	30.72572188260947	-22.85981549916443	4.89413477926751
C	33.59197477869114	-22.60896279642709	9.44306863816039
C	38.85992595459525	-28.58189441677235	9.14799848964726
C	36.54492324251481	-30.21191130841448	1.66255171333699
C	32.63474700299924	-25.86948431655562	3.76031229573858
C	33.95878125637220	-24.42369420409091	7.58999311315022
C	36.89825687939037	-27.58420343027027	7.72243191577750
C	35.86951128811548	-28.72184428684561	3.71059620865176
C	31.57524613941295	-24.89620370019674	3.53692573081522
C	34.25520990365501	-23.83524905847493	8.88768856808470
C	38.03286560485898	-28.48186607208306	7.90016205138755
C	35.64944931094941	-29.23327518805574	2.36508785794400
C	31.59365500214524	-24.05092168020666	4.61360238281630
C	35.22965499046139	-24.61614934217789	9.44972780786062
C	38.17555890142725	-29.15576024813947	6.71877145786662
C	34.50737011140306	-28.63239072288702	1.90841043861523
C	32.65496040783918	-24.52709553536367	5.48897095595404
C	35.52330822815187	-25.66450765984472	8.48245444061080
C	37.11402207350910	-28.67783497159605	5.84418420991782
C	34.06560208028812	-27.73612697865906	2.96898650600739
N	36.35544042038551	-27.73882001838327	6.48017737804135
Fe	34.77146763090263	-26.71981173861502	5.73830533685706
C	34.25707309376282	-31.46461305614385	5.94069868489775
C	33.76621628824097	-31.84980861767937	4.55085432829389
C	32.38856546330457	-27.36424448190753	7.50154714012039
C	33.44653308475316	-27.90876586255598	6.57474126169116
C	33.25012418133124	-29.34984376118048	6.35350592147866
O	32.16596691772477	-29.92499784584131	6.37484571447675
O	34.39590049081290	-30.05002492511911	6.11059814344357
H	29.99017585990246	-22.70042323815002	4.09795426916417
H	31.31576867105045	-21.93711536168514	4.98437543404760
H	30.16881453611022	-22.97392763797630	5.83467563682639
H	31.25651855536703	-24.73973520816168	1.40329014451508
H	30.10694967778097	-25.79575260481987	2.22685645991134
H	29.96328145343020	-24.04054005742189	2.38483546107024
H	33.74487975585568	-27.84633604928857	0.04352262408523

H 34.35675409380148	-29.50135418257772	-0.06019527557565
H 32.79547727449683	-29.17992711360544	0.70468503053369
H 36.20463720695434	-30.4031657264698	0.63902540605872
H 37.57696150843326	-29.84054642235293	1.60123202827938
H 36.58534095710684	-31.18133436869348	2.17909506350088
H 33.99300743372817	-22.34779309931383	10.42858134139664
H 32.50741413650303	-22.74640551920364	9.55679378334922
H 33.73522051429023	-21.73795372597138	8.78862808764738
H 36.99909998540573	-24.30704022565673	10.65412688443537
H 35.79148577322120	-25.34822375736813	11.40848858363676
H 39.66066679882094	-29.32159605909107	9.03974523750885
H 39.33224603679881	-27.62277988427564	9.40271754669391
H 38.25519097988276	-28.87940675170247	10.01637320599100
H 38.73600933846863	-31.13981218463915	6.05898751576337
H 39.79760602015312	-29.85754722263977	5.47356285557982
H 39.89611095739320	-30.38394267446058	7.15802671388981
H 35.52535600267373	-23.60246528722486	11.33212300541178
H 34.40428787442571	-31.41153540721242	3.78093961819423
H 33.77636450192431	-32.94066201122918	4.43553470722204
H 32.74735253865276	-31.49281080452673	4.39948473159638
H 33.57947607416207	-31.85524076015376	6.70541208601433
H 35.26190614112103	-31.85437189249095	6.12220397382697
H 32.82751308118500	-27.17362373574117	8.49156959561991
H 31.99172819580492	-26.40646143833219	7.16074067433177
H 31.55811085231489	-28.06396026943851	7.62902588085713
H 32.40153136683924	-26.92565441710493	1.94151282839120
H 37.02771057434726	-26.63738781646284	9.61137727293120
H 37.61663516105592	-29.84356714927400	4.14666243390191
H 32.42699793781988	-23.07217580085259	7.01695381310274
S 36.40910450994762	-25.25840749228643	4.65580607400688
C 36.05169561402440	-23.50547851855743	5.05589265085850
H 35.06616599443672	-23.19816373222805	4.68761037408530
H 36.08470862111408	-23.32006188501759	6.13562156135840
H 36.80950295159369	-22.87448642735425	4.57615823624254

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B3LYP Scan/Thiolate IPC Model/BSS/40 degrees Constrained Optimization

C 30.71430010969492	-24.73372207875233	2.29676681539738
C 35.87504387777875	-24.54557466604492	10.79211856988381
C 39.15133618907312	-30.20462634505078	6.25933028417195
C 33.74050509277566	-28.75352617164303	0.55417510674377
N 33.26048360084277	-25.57495820164805	4.92367980217874
N 34.72532401422107	-25.52689161261075	7.35608903027418
N 34.86438279728269	-27.79036187963317	4.00396334454659
C 32.96861213583158	-26.79030734334399	2.81746517117248
C 32.98618236382725	-23.93003872612794	6.71617423192904
C 36.46555293437950	-26.68229801762794	8.63641798919734
C 36.86427697654365	-29.11015809792735	4.48331407786036
C 30.76284760968798	-22.77178493040710	4.89321627745089
C 33.57064276291125	-22.65424739804028	9.48239006007272
C 38.82063664156937	-28.63808297705983	9.09261389437271
C 36.43734095734295	-30.22695943494522	1.61992480824468
C 32.63566550253272	-25.79279895847390	3.72857389549251
C 33.94476691988523	-24.42915996402994	7.59273898889375
C 36.87323571875896	-27.60149663017982	7.67557720022740
C 35.81494292789336	-28.70854924083800	3.66276565247045
C 31.59434619851726	-24.79865017373244	3.51015730187279
C 34.23349193774771	-23.87066032247924	8.90532792072934
C 37.99951066091923	-28.51175012973951	7.84344386679639
C 35.57342483583122	-29.22015458301506	2.32121969947371
C 31.61546963295020	-23.97104702156932	4.60031771114885
C 35.19973475055257	-24.66823695707679	9.45785661588357
C 38.13856554941430	-29.17086432751629	6.65341648888831
C 34.44282874319109	-28.59498525549247	1.86983921535293
C 32.66146951619788	-24.47731198760601	5.47709739882168
C 35.49708202492095	-25.69605192781225	8.46990582421466
C 37.08228627696123	-28.67200302788758	5.78402345817628
C 34.02705630711026	-27.68631889488866	2.92994008736079

N	36.33419918957343	-27.73221015174221	6.42923298053353
Fe	34.75337096015338	-26.69865304017307	5.70455771065907
C	34.34573861547954	-31.47964060972072	6.28705672473900
C	34.20593146331997	-31.99282315124536	4.86000239502315
C	32.32254330230254	-27.37423365909011	7.38153781579184
C	33.44077693846616	-27.89546701550141	6.51275575368884
C	33.29421217058773	-29.34700334423767	6.30797081112049
O	32.22971686640902	-29.92161039119911	6.11726577390794
O	34.46185961498131	-30.05317750920979	6.36212541387765
H	30.03628679917439	-22.58825410230986	4.09397178794040
H	31.36565732781310	-21.85956578591813	5.00354145062936
H	30.19648989556064	-22.89306872325178	5.82721728716203
H	31.29992177407537	-24.59991223521119	1.37673532261784
H	30.12708484430732	-25.65386251154871	2.16951069984107
H	30.00638956542115	-23.89989297045203	2.35748569637216
H	33.67456668184757	-27.80102908963049	0.01056249937009
H	34.26192120506978	-29.46463054582727	-0.09574210697754
H	32.71214047048455	-29.11943432263182	0.68278269109554
H	36.08335179668995	-30.41856813706904	0.60106177794321
H	37.47837998370090	-29.88380462009132	1.54605130356841
H	36.45706706748083	-31.19271483255408	2.14471972889174
H	33.96726416025869	-22.41454138458080	10.47512303826470
H	32.48502569690883	-22.79058996275917	9.58754766787154
H	33.71977806593001	-21.77042001291912	8.84669215174647
H	36.95940046234039	-24.40262983930959	10.68663777456822
H	35.73258414263498	-25.44524415901321	11.40710110042927
H	39.61627181957369	-29.38203327587686	8.97599280268612
H	39.29903443635700	-27.68683497733505	9.36484520202028
H	38.20982354796964	-28.94499519281264	9.95350677600181
H	38.67695936425505	-31.15413861703241	5.97434884628875
H	39.75079592620211	-29.87784459472115	5.39820549222821
H	39.84735603875493	-30.42056992561126	7.07764228082806
H	35.48610063443322	-23.69539248300002	11.36314939438583
H	35.03693489131290	-31.64459912623126	4.24394324645496
H	34.20058995097640	-33.08970728238595	4.85329677167646
H	33.27461188804608	-31.63737043928539	4.41899204501164
H	33.49354407896119	-31.80250914897196	6.89143885871944
H	35.26730895246997	-31.84738477419776	6.74545148644002
H	32.67601376857909	-27.28018792335800	8.41996564994179
H	31.98785680676882	-26.38052219753780	7.08513139963296
H	31.46232279560547	-28.05093833692218	7.38347455126343
H	32.38610861567047	-26.83191292150117	1.90198056128742
H	36.99641368077162	-26.69334493532692	9.58383675181510
H	37.55654845046953	-29.84448916329334	4.08204261260483
H	32.43223680352016	-23.05113530584487	7.03194543769291
S	36.42071483004550	-25.24026664566723	4.65889361822336
C	36.03486157803260	-23.48510839162461	5.02215492859595
H	35.05625916121456	-23.19345655845082	4.62381865589080
H	36.03739562563587	-23.28353575018635	6.09955192269525
H	36.79841841125481	-22.85244274242791	4.55375907363848

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B3LYP Scan/Thiolate IPC Model/BSS/50 degrees Constrained Optimization

C	30.72700552405921	-24.61720474264915	2.30251354264805
C	35.90865361436453	-24.60367703743431	10.78816662989115
C	39.10651204602305	-30.24234616787352	6.17140504491238
C	33.65780132249533	-28.69409641596994	0.52605181867627
N	33.26047423322132	-25.53107857634518	4.91846739809451
N	34.72653278483308	-25.53919145766854	7.35030782524634
N	34.84083633769916	-27.74829715033685	3.96050749183710
C	32.95810642617083	-26.70625113254078	2.79036828496029
C	32.98257537281036	-23.93037291192208	6.74824550082089
C	36.48450469282672	-26.70494294925230	8.59523687528481
C	36.80375756864590	-29.12471463520975	4.42977507076250
C	30.77185376879336	-22.71923540936971	4.94623835562792
C	33.58198184058465	-22.70373776414727	9.53266628129628
C	38.83319948309908	-28.67375442667529	9.00944291777810
C	36.30404286453672	-30.26061254186248	1.58487034348409

C	32.63755930199743	-25.71872863250859	3.71724276854278
C	33.94457480697538	-24.44732777911447	7.61152309024883
C	36.87532159354625	-27.61789056856590	7.62235879252471
C	35.75834429377327	-28.69860857898788	3.61646316915938
C	31.60152366400827	-24.71482378911951	3.51763937144606
C	34.24415670412763	-23.90801944154959	8.92997544721498
C	37.99512002328124	-28.53884249055438	7.77249934338572
C	35.48819909219532	-29.21124240486373	2.28079183052557
C	31.62040330942607	-23.91506275411318	4.62846319763094
C	35.22104420936357	-24.70833190203813	9.45879030509175
C	38.10920677266341	-29.19965776669999	6.58107613447186
C	34.37790280246308	-28.54851359176452	1.83348325405483
C	32.66164662659953	-24.44570537953830	5.49563942596125
C	35.51135951395388	-25.72028533744504	8.45305403859294
C	37.04590665124951	-28.68800337630293	5.72743884352998
C	33.99807902032866	-27.62392063862997	2.89293241626744
N	36.31830712977915	-27.73920463949582	6.38242752648201
Fe	34.74453510355513	-26.68303086567422	5.68060199116947
C	34.30281349484468	-31.47945883195509	6.68493173824118
C	34.74718604492526	-32.07239044671874	5.35510332765591
C	32.14765057702845	-27.41010626256657	7.04954694649437
C	33.43103326973111	-27.89042570322273	6.41415706907959
C	33.35782716659605	-29.34788342634134	6.19556924709917
C	32.42979042298061	-29.92171452622477	5.64929169776993
O	34.40732649375065	-30.04761579972779	6.72598323809818
H	30.03783873052783	-22.52408838116044	4.15658334105430
H	31.37653513370593	-21.80896764771221	5.06306540798851
H	30.21431248186775	-22.85262410813273	5.88382985946580
H	31.31540875757172	-24.44806209389859	1.38999726189699
H	30.14860998600234	-25.53771463340074	2.14204651668327
H	30.01149956401192	-23.79196170507418	2.38716198763313
H	33.59573975261922	-27.73875955084482	-0.012850905057668
H	34.16371130943062	-29.40799183399263	-0.13300112784261
H	32.62725255632019	-29.04949015544559	0.66633581608147
H	35.93515635908246	-30.44826841190932	0.57049933328512
H	37.35871126823692	-29.96439399275419	1.50002333380967
H	36.28371632761878	-31.21916148797896	2.12222842097765
H	33.99053718532624	-22.47566670608384	10.52330596941484
H	32.49850422507222	-22.84719125912056	9.65019994302415
H	33.71800553971293	-21.81018194664469	8.90765241874420
H	36.99333721493930	-24.47037316302444	10.67455365629043
H	35.76257204067724	-25.50731765888116	11.39655808045400
H	39.63210694169744	-29.41106025737531	8.87441913952440
H	39.30878219159303	-27.72224488012352	9.28530392142739
H	38.23603928924182	-28.99386061291323	9.87513293631632
H	38.62292140271575	-31.19499103578011	5.91287211411161
H	39.68175813884887	-29.92824676296210	5.28944913048629
H	39.82534499816041	-30.44948860711722	6.97213026207206
H	35.53302412929751	-23.75460003380709	11.36977850499187
H	35.76335301311302	-31.75413894735322	5.11475236763181
H	34.72512164304342	-33.16781697637997	5.40636557143176
H	34.08392283364715	-31.74691005313835	4.55317952213516
H	33.27175176254561	-31.76883528762658	6.90505931957403
H	34.95104212320983	-31.81660851764515	7.49802586316465
H	32.24473282147285	-26.41293402189412	7.47231978964324
H	31.34996443714422	-27.37489970584590	6.29364104306684
H	31.79107957397952	-28.08769832601489	7.83926312529085
H	32.37225621225547	-26.72926767888377	1.87637892726156
H	37.02870340458431	-26.72448152827964	9.53486484507113
H	37.47591768519865	-29.87455848866436	4.02319098763875
H	32.42938975890640	-23.05873957175358	7.08478058365899
S	36.43231631582452	-25.20787016472678	4.66423649383520
C	36.00519939480895	-23.45395547569018	4.98745754369019
H	35.02930116345851	-23.18870884188830	4.56481467675949
H	35.98241626874855	-23.23304118581941	6.06098079089669
H	36.76493677947351	-22.81380014927798	4.52288008587565

B3LYP Scan/Thiolate IPC Model/BSS/60 degrees Constrained Optimization

C	30.64471083796580	-24.56417819726255	2.26277670207509
C	35.48200443160896	-24.56616278257176	10.95198463552988
C	39.12695557194017	-29.91665099560715	6.31579758321332
C	33.84598076328590	-28.43292477172183	0.48850044087976
N	33.08876658298729	-25.46662880781904	4.96721807769996
N	34.47243120393335	-25.46346433884092	7.45003605173983
N	34.84007041750399	-27.54927780395982	3.99868811298586
C	32.95053769139029	-26.56646435631892	2.78498910927376
C	32.68019935268516	-23.92323148834778	6.81996047251637
C	36.24915959650595	-26.56758450764432	8.72198922541537
C	36.83386614387307	-28.86753397102539	4.51397893190591
C	30.49010144546755	-22.75772002184450	4.96308116575257
C	33.11339119866544	-22.74753538969811	9.65729208184444
C	38.67794231394657	-28.42841362369458	9.17381822487159
C	36.49839310210218	-29.93643518703092	1.61978109163774
C	32.53403957995150	-25.63627391728618	3.73115860442191
C	33.63242283005749	-24.41807756018957	7.70735492929244
C	36.72799149977227	-27.42607487846562	7.73762196732281
C	35.80735871355244	-28.45738962224243	3.66884586812967
C	31.46416386018794	-24.67043244232051	3.51504533829230
C	33.85519004261291	-23.90178580281481	9.05045812262351
C	37.88109110031170	-28.29953239949893	7.90915223675644
C	35.61346267254166	-28.94004183390173	2.30938081221901
C	31.39998912204420	-23.90826339327262	4.64921926378519
C	34.84945551631758	-24.66765251557983	9.59564649818147
C	38.06943839824753	-28.92761428459576	6.70849725367856
C	34.49782263985808	-28.30597377213140	1.83326352882291
C	32.42449391848500	-24.42362920205332	5.54667037848536
C	35.22820354902176	-25.63444253252181	8.57405054318200
C	37.01782646206870	-28.44274235469869	5.82587765422091
C	34.03413776877151	-27.43215020826019	2.90183573194048
N	36.22827800442129	-27.53671486086213	6.47204235004805
Fe	34.61976845425752	-26.55366778691053	5.74490254205043
C	34.36673601832411	-31.41022873154150	6.65743669219414
C	34.97103562128498	-31.93917980547021	5.36422867558261
C	32.09731107943930	-27.50413523493287	7.13968896340072
C	33.37305487594287	-27.85089605390721	6.4138680862828
C	33.39072588650660	-29.30199469217444	6.13167698880145
O	32.55930705700995	-29.88873592565832	5.46141015329525
O	34.40518570661467	-29.97673895225484	6.75453752816089
H	29.77491924810799	-22.57623678269794	4.15299756420549
H	31.05068790698879	-21.82552415964563	5.11958434910928
H	29.90842330529162	-22.93626853611087	5.87827258866987
H	31.26291812619261	-24.30110510387970	1.39288856811707
H	30.14219744951420	-25.51125655049663	2.02185342355348
H	29.86901297442538	-23.79603579153551	2.35516457895226
H	33.78430631186278	-27.46410054456715	-0.02608780186753
H	34.40188704857961	-29.11433656444363	-0.16476755147840
H	32.81998679389272	-28.81844896762306	0.56789163393266
H	36.19865358039859	-30.08475511711012	0.57653918239873
H	37.54812158766963	-29.61212537100511	1.61520585476032
H	36.47032286148038	-30.91940903423077	2.11090892433152
H	33.45068991669618	-22.54638585826508	10.68007521737179
H	32.03095807759283	-22.93373976915870	9.70005564203371
H	33.25455093747667	-21.82483106294691	9.07746976421526
H	36.55236780860240	-24.32654439085715	10.88435278345449
H	35.40232754068732	-25.50913059849532	11.51089684666866
H	39.50516480865436	-29.13686998193996	9.05588340488944
H	39.11048171122215	-27.46693871050780	9.48376165238274
H	38.05987530523759	-28.78376624612687	10.01046665829278
H	38.69643532448094	-30.88044701506680	6.00940757366693
H	39.72727101464704	-29.55465939127692	5.46937063574747
H	39.81745273154519	-30.11815343914329	7.14239216222534
H	35.00964625156659	-23.78605561581335	11.55894934567223
H	35.99775369067193	-31.58795387116527	5.24533593336864
H	34.97538958981491	-33.03597686776993	5.37372196708565
H	34.38908766921740	-31.59985717292045	4.50692035541015

H	33.33097082606804	-31.74574513497152	6.75625096895657
H	34.93776931172974	-31.75332952543001	7.52398877273944
H	31.97147772983595	-26.43587043516172	7.29147856719804
H	31.23046102724748	-27.88377167707290	6.58089743726753
H	32.06410523987271	-27.99158736116642	8.12830584205511
H	32.40845911846507	-26.58527837809011	1.84429791152161
H	36.75749607123197	-26.59020862070740	9.68149574468551
H	37.54517270134683	-29.58750566365680	4.11997530001714
H	32.07891985753077	-23.08300404365952	7.15406311061053
S	36.08892386750730	-24.75193517367439	4.96099058833999
C	37.48287592672035	-25.44895600845727	3.99460605712606
H	38.12031765205774	-26.09700505607925	4.60713547328570
H	37.12925918644567	-26.03120485721355	3.13604200395693
H	38.09738756495543	-24.62239064292577	3.61791283021178

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B3LYP Scan/Thiolate IPC Model/BSS/70 degrees Constrained Optimization

C	30.62991123659278	-24.61212824545841	2.28439195405224
C	35.53432077257770	-24.49386763165435	10.93682510656577
C	39.13330678302290	-29.92170093151839	6.35761694982129
C	33.88036126299931	-28.43802896558757	0.50495828567094
N	33.09395634802805	-25.47631381137392	4.98274396653705
N	34.48571754718004	-25.45228727176438	7.46224406713508
N	34.85644765749156	-27.55393538132905	4.02006272425130
C	32.96804454116491	-26.57787836930980	2.80039886932372
C	32.67217211643574	-23.93564819704412	6.83398271641826
C	36.28003588990916	-26.52993235832236	8.73233919859819
C	36.84043409081350	-28.88152030879198	4.54931416141508
C	30.45173216107617	-22.81067895689698	4.98622811075526
C	33.13233713553073	-22.71505369908291	9.64758746313732
C	38.70901817773171	-28.38770166520587	9.19438575425210
C	36.52600148583235	-29.94276682193374	1.65027811437449
C	32.53985081132681	-25.65420099702069	3.74743876501085
C	33.63979280860571	-24.41019672157792	7.71571022989792
C	36.74944816141129	-27.40470545822119	7.75806961717539
C	35.82219356762079	-28.46579168278038	3.69689430466493
C	31.45438797857400	-24.70534567171798	3.53446861777101
C	33.87456376274707	-23.87331362788557	9.04888414515164
C	37.90216018950266	-28.27746358933804	7.93422360665606
C	35.63623514724506	-28.94780948024933	2.33602820852087
C	31.37980758522214	-23.94580613927420	4.66980083566199
C	34.88243420920340	-24.62264197778380	9.59194736515122
C	38.07998011955089	-28.92506507278515	6.74232377506002
C	34.52470836299651	-28.31153908675079	1.85328190086000
C	32.41478404313295	-24.44499976741228	5.56458739933509
C	35.25522142913119	-25.60177315780133	8.57984662940314
C	37.02451314394057	-28.44998610867962	5.85903123833734
C	34.05585799512440	-27.43767763105491	2.91961078118675
N	36.23987160844680	-27.53364537669763	6.49771279738725
Fe	34.63075757044796	-26.55262562096190	5.76290993390607
C	34.15604057668413	-31.46533114745026	6.49773868107002
C	34.92412584814635	-31.92285349767258	5.26638790039175
C	32.15322478820848	-27.53325630976745	7.22801380107638
C	33.38411965113838	-27.84612456180636	6.41540212538904
C	33.35437809996465	-29.27110932851899	6.02032256558069
O	32.58321036028698	-29.75402761924379	5.21299190207297
O	34.24421679224977	-30.04657752847547	6.71452453636522
H	29.73206631132319	-22.64074942537462	4.17758095718055
H	30.99713739303595	-21.86933144549109	5.14181573507997
H	29.87488423200516	-22.99887580345608	5.90256977024284
H	31.24085493127902	-24.33643281782251	1.41323779405616
H	30.14431167202413	-25.56792627510896	2.04339420932387
H	29.84064980286263	-23.85834083408102	2.38013483117054
H	33.81767672327165	-27.46852201418791	-0.00813700438651
H	34.44200275470689	-29.11629198673910	-0.14674776702697
H	32.85556272167180	-28.82771763564308	0.57899203844428
H	36.23812388855048	-30.08280547450499	0.60253500249467
H	37.57653279166101	-29.62134206442526	1.66025469307174

H	36.48977412594543	-30.92935247523424	2.13366206496579
H	33.47802975465252	-22.49893680046339	10.66450556816417
H	32.05130214805862	-22.90609769438520	9.70290611050177
H	33.26334162538591	-21.79934368870208	9.05442724542924
H	36.60042100480190	-24.24203486397650	10.84897494477573
H	35.47526970263952	-25.42934121821236	11.51067167609336
H	39.53401563322097	-29.09947871078621	9.08098556529254
H	39.14589602815339	-27.42216635764023	9.48507461573644
H	38.09734404592436	-28.72827657993770	10.04178446400904
H	38.69890128408674	-30.88784610016388	6.06427127537465
H	39.73182872360920	-29.57178564626360	5.50482443030587
H	39.82618971554614	-30.11518120709831	7.18414438278647
H	35.06162151674199	-23.71077668936655	11.53969061583688
H	35.97311347142256	-31.62686348669575	5.33159611938620
H	34.87274655295472	-33.01471295838145	5.17607498712186
H	34.49807039886494	-31.47670253633207	4.36735528206000
H	33.10339843405441	-31.74807183206132	6.41683457260194
H	34.57475821803096	-31.90427945961385	7.40703989171392
H	32.08684779267674	-26.48598596277360	7.51084865072224
H	31.24812082904013	-27.79908670109989	6.66218520827744
H	32.12876307081323	-28.13579014644640	8.15105111133219
H	32.42714593563606	-26.60111808090995	1.85914615908247
H	36.79762498728774	-26.53646278777125	9.68712143304589
H	37.54865447774163	-29.60773588800473	4.16137148689135
H	32.06267523808039	-23.10106401774717	7.16744002142970
S	36.09818451722510	-24.75299571977245	4.97192413870522
C	37.46978574379651	-25.45229527142858	3.97489800954384
H	38.11888384836168	-26.10185657506790	4.57352278385376
H	37.09738112118153	-26.03325603415994	3.12348814812917
H	38.07791169937528	-24.62673905646705	3.58575407778818

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B3LYP Scan/Thiolate IPC Model/BSS/80 degrees Constrained Optimization

C	30.66625203483580	-24.42247927409579	2.22761642912652
C	35.46170972959093	-24.71066325695435	10.93488665352380
C	39.08974533090265	-29.95676616011570	6.15907408559134
C	33.81912049148502	-28.29275507787852	0.37193718137623
N	33.08323104331217	-25.42777788968279	4.92029019925280
N	34.45773026714259	-25.50423121244940	7.40646014755062
N	34.81969140755371	-27.49958489265467	3.90183392628412
C	32.95452987786668	-26.45618929998875	2.70274401343806
C	32.65936573560879	-23.95219176108640	6.82371027281887
C	36.24213590728321	-26.63633940170973	8.64438800969808
C	36.76954445686639	-28.88759840501298	4.40145378889257
C	30.48982152346940	-22.71434560650020	4.98961435974496
C	33.07514645852833	-22.87441986295631	9.70128480255266
C	38.67604144196412	-28.50350809397688	9.04274015540804
C	36.41142502066148	-29.90253745936765	1.49334964828382
C	32.53894334800398	-25.55195833491244	3.67431533402975
C	33.60897823298518	-24.47510986848440	7.69772259456241
C	36.71256642316892	-27.47866522912399	7.64182589839018
C	35.75834506802136	-28.43258386382575	3.56162275829223
C	31.47345842109845	-24.57601520931706	3.48281841440074
C	33.82768548676221	-24.00096556398328	9.05680987831008
C	37.86168021290240	-28.36103242858397	7.79066649753101
C	35.55743521980867	-28.88664541458340	2.19297702017794
C	31.39988054142956	-23.85526540321214	4.64306961895270
C	34.83054455825854	-24.77366288607720	9.57570412468954
C	38.03219761084178	-28.97902246737537	6.58102582868090
C	34.46700064588699	-28.20912207255906	1.72177224649974
C	32.41569286023196	-24.40447945739378	5.53034652513154
C	35.21634326915480	-25.70479753032003	8.52405762925133
C	36.97275644568972	-28.47871362053970	5.71629243397870
C	34.02211751151481	-27.34239739993177	2.80472357185416
N	36.19987810932893	-27.56987410414996	6.37958700555961
Fe	34.60265867965700	-26.54699047535637	5.67124146910182
C	34.22363205502725	-31.36106175319196	7.08120869468470
C	35.39261055530945	-31.88573488249621	6.26218944335154

C	32.03631794659643	-27.55888626891301	6.94912259264272
C	33.36329510407501	-27.85274656757315	6.29808106381629
C	33.49214414776127	-29.31117908310765	6.08991447288385
O	32.98953161676003	-29.94542345146612	5.18440264629312
O	34.18097686269807	-29.92458783791660	7.10638762169279
H	29.77030128470156	-22.51426032587475	4.18775635524665
H	31.04967350170737	-21.78511672615315	5.16581846368025
H	29.91310274499676	-22.91593933461779	5.90309891137857
H	31.28693196174167	-24.09687382545334	1.38076814590725
H	30.19111438069094	-25.36729800729534	1.92947411674521
H	29.86984814187900	-23.68032505424706	2.35137579825191
H	33.79087293804026	-27.31415227310353	-0.12700571435131
H	34.35670173113414	-28.98078079361522	-0.28963324891880
H	32.78111741113602	-28.64711761503501	0.44009700935067
H	36.11742587823280	-30.01999998790393	0.44453385590018
H	37.47289102576342	-29.61921683826309	1.5050912203178
H	36.34026038547552	-30.89273259861617	1.96526174643108
H	33.40203609608393	-22.71150987817051	10.73421167327460
H	31.99337970385585	-23.06725152680454	9.72687775296065
H	33.21657727252660	-21.92889488282609	9.15943514289900
H	36.53137417568664	-24.46582356375640	10.87528632624598
H	35.38459855375569	-25.67017667226148	11.46533449981124
H	39.49405528879130	-29.22001813307810	8.90999424218380
H	39.12288176109892	-27.54775776197196	9.35001850275702
H	38.06651678054816	-28.85588051635182	9.88673679030214
H	38.66080316897708	-30.91684806667006	5.83979449863739
H	39.67743192643425	-29.57507659063153	5.31256083522173
H	39.79117174640798	-30.16911496028680	6.97372409062414
H	34.98661497747312	-23.95038802461434	11.56448036690041
H	36.33287440027797	-31.46863251053321	6.62894613780082
H	35.44180940998513	-32.97937283065647	6.32784444612055
H	35.27808825411560	-31.60307853924308	5.21493788459138
H	33.27684636680755	-31.74069197067925	6.68969965892386
H	34.31914919587118	-31.65093500262850	8.13111967037876
H	31.87671142765688	-26.49778281151308	7.12322855469291
H	31.21364151727408	-27.93225440033738	6.31981012967385
H	31.94840843542782	-28.08193708482745	7.91527241013640
H	32.41911259450130	-26.44122907636578	1.75812837840357
H	36.75540685945604	-26.67913423978209	9.60054136898365
H	37.45808431458075	-29.62398860740024	3.99807159717593
H	32.05419480105848	-23.12591037334950	7.18449906797039
S	36.07871373490791	-24.74037451016602	4.91626282268165
C	37.50192421394450	-25.44335195878735	3.99766011976793
H	38.11872925558603	-26.08995670629054	4.63256314725139
H	37.17426709825387	-26.02826560725772	3.13066101789389
H	38.12968030811037	-24.61952108375533	3.63710765177980

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B3LYP Scan/Thiolate IPC Model/BSS/90 degrees Constrained Optimization

C	30.67013054049706	-24.37650634248497	2.21148315780990
C	35.45294832791826	-24.76186452822571	10.92125300216589
C	39.06041714136671	-29.98764269888864	6.10231480142505
C	33.80521298261316	-28.24755667955909	0.32677581508937
N	33.07543533062786	-25.42072207907982	4.89981125045554
N	34.44958782820956	-25.52183689924475	7.38509421096810
N	34.81379032090729	-27.48027918736393	3.85999643851705
C	32.95080002078641	-26.42286681967136	2.67006918144515
C	32.64911617666677	-23.96609171739904	6.81889500533377
C	36.23686324924965	-26.66275321981979	8.61088556293015
C	36.75314152051424	-28.88542076311926	4.35071761602430
C	30.48891499289190	-22.70129555802355	4.99331974268595
C	33.06305488259640	-22.91767492874929	9.70678182452396
C	38.66567618231505	-28.54004092034081	8.99356977668692
C	36.38629896382538	-29.88190110394216	1.43811134047934
C	32.53474886878439	-25.52852719060368	3.65078591001752
C	33.59866742329595	-24.49765075029556	7.68747402262261
C	36.70526550988922	-27.49779235322612	7.60135142653323
C	35.74605834214192	-28.41680442341068	3.51381050873700

C	31.47200376880157	-24.54813768044670	3.46771413723949
C	33.81721570540068	-24.03663419579687	9.05098001245678
C	37.85030495393406	-28.38660405011881	7.74328975739182
C	35.54166545554470	-28.86174692531986	2.14259802082525
C	31.39608684947878	-23.84136760558950	4.63644870429289
C	34.82209648270014	-24.81227359966125	9.56142777711299
C	38.01544715688248	-28.99930000266764	6.52989481490890
C	34.45548666859674	-28.17487771936722	1.67605132384466
C	32.40778942903747	-24.40339393826144	5.52001840236981
C	35.20939115613512	-25.73186649504668	8.50018064021499
C	36.95831136265837	-28.48804578485051	5.66899206439419
C	34.01604295900915	-27.31234901676799	2.76479173310735
N	36.19082200570418	-27.57902404867822	6.33884449136345
Fe	34.59588201259564	-26.54650531110517	5.63835532491799
C	34.20190944901547	-31.33077817651970	7.22749789477196
C	35.49639262631993	-31.82150498680629	6.59739882771003
C	32.04251389719214	-27.59225607219918	6.92163858895598
C	33.36719626124238	-27.86516366851497	6.25843612060335
C	33.55462041575119	-29.32319030264565	6.09469679949138
O	33.21634504731489	-29.99030936348246	5.13915008508333
O	34.10445006253114	-29.89707299195701	7.21665267200184
H	29.77185875959632	-22.49016812232898	4.19209728679256
H	31.05163701445210	-21.77592222562494	5.18044655510655
H	29.90954406433178	-22.91039821202152	5.90343445451049
H	31.29451560810151	-24.03937478700209	1.37189802933683
H	30.19563131081949	-25.31666964112216	1.89796098812339
H	29.87357287607874	-23.63572218774980	2.34229988277176
H	33.78362764777735	-27.26664499574818	-0.16803897722449
H	34.33657087256053	-28.93689463713345	-0.33841510603301
H	32.76459140239808	-28.59429339514494	0.39476576546793
H	36.09221753188455	-29.99069592138008	0.38837011776504
H	37.45062698679940	-29.60972646838462	1.45245543147731
H	36.30380478625712	-30.87361396966564	1.90484268539914
H	33.38953888725068	-22.76467449581265	10.74134906873576
H	31.98151541906398	-23.11198623712682	9.73024172362843
H	33.20343959855730	-21.96650242268013	9.17460586037083
H	36.52262453075940	-24.51649103958538	10.86432868994835
H	35.37552698484379	-25.72620252336444	11.44286720609736
H	39.47891447149448	-29.26114600425663	8.85637199196425
H	39.11907675734304	-27.58848651718434	9.30424879160051
H	38.05535606542089	-28.89208723784244	9.83706610769574
H	38.61703749093264	-30.94278456118266	5.78782815601094
H	39.64682752009325	-29.61370388242468	5.25158168192354
H	39.76454702495808	-30.20690756097978	6.91284543284797
H	34.97763654375515	-24.00743049101110	11.55769079064180
H	36.35809759084181	-31.36210078194224	7.08654365703273
H	35.57535625799460	-32.91132491181160	6.69187232872269
H	35.52518080014672	-31.55902243961419	5.53914571306332
H	33.33653521693696	-31.75246363047791	6.71076707266927
H	34.15448116308212	-31.60167731927642	8.28588355454990
H	31.86210507923246	-26.53195954070542	7.08131518576286
H	31.21733023603729	-27.99006172073931	6.30942160287218
H	31.97990114795232	-28.10332244514512	7.89537390434303
H	32.41667925264898	-26.39719245278598	1.72492052685809
H	36.75110639026400	-26.71352733475174	9.56611254220864
H	37.43643655100032	-29.62391017931632	3.94229193396597
H	32.04348529858711	-23.14396757036439	7.18829666152490
S	36.07005078064582	-24.73291985477058	4.89929032922622
C	37.51105889868142	-25.43500800490898	4.00826625010179
H	38.11708228123815	-26.07878579579686	4.65629684087636
H	37.20029417959467	-26.02281589869201	3.13707282086415
H	38.14396307364047	-24.61106258289188	3.65714207888990

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B3LYP Scan/Thiolate IPC Model/BSS/100 degrees Constrained Optimization

C	30.66153843491308	-24.38465625716815	2.21147391011879
C	35.45057140723890	-24.78000515915434	10.91739474374547
C	39.05093591138813	-30.00573156136058	6.09253904908059

C	33.84165671063403	-28.20533675496778	0.29781871191673
N	33.07865584133941	-25.42109385771747	4.89174576792963
N	34.45140517353188	-25.52842344585244	7.37761570124017
N	34.82666389314353	-27.46753900730231	3.84413807402980
C	32.96298358937622	-26.41033874723711	2.65575459771354
C	32.64485908394933	-23.97749636674073	6.81756173489307
C	36.23715164504114	-26.67327210052647	8.60257709772178
C	36.76392611358084	-28.87631499210050	4.33352850703351
C	30.46838515435493	-22.72550779565935	5.00246580943377
C	33.05728893400430	-22.93648490268906	9.70855107341310
C	38.66246868187651	-28.55637524069859	8.98409606621344
C	36.42154547757669	-29.84119590639500	1.40959386170354
C	32.53845693413915	-25.52648796610293	3.64225964731013
C	33.59829533200621	-24.50696521679008	7.68324436807894
C	36.70521469161523	-27.50726893030609	7.59208840006250
C	35.76299495349354	-28.39865865205843	3.49491921856034
C	31.46711257104912	-24.55451073549870	3.46558067085872
C	33.81510082109450	-24.05043763371296	9.04848671670753
C	37.84798197051946	-28.39908484088292	7.73361426458353
C	35.56857550434692	-28.83106698674566	2.11837292746363
C	31.38622864221372	-23.85456817967347	4.63813821947022
C	34.82121903533970	-24.82596132590559	9.55673049771829
C	38.01319171787859	-29.00967237414152	6.51907970910188
C	34.48273046806861	-28.14386531337922	1.65201402063743
C	32.40371457557232	-24.41226866235786	5.51780835796560
C	35.21058913415072	-25.74125429305245	8.49267211040712
C	36.96092665874859	-28.49174554939023	5.65671474091844
C	34.03383140006529	-27.29349676347927	2.74667215832913
N	36.19246159214776	-27.58443018070410	6.32839831827856
Fe	34.59986294894298	-26.54596495409119	5.62632159322556
C	34.11204916703795	-31.34499727405753	7.23883308506852
C	35.46805263111884	-31.79621754382801	6.71615447666700
C	32.07595298690659	-27.59403081424556	6.96830894249428
C	33.36900480871417	-27.86694000457352	6.24574901734593
C	33.56494573745486	-29.32222896911466	6.07830401218542
O	33.34750343649454	-29.97699305903038	5.08069363535661
O	33.98389311494115	-29.91417303305226	7.25010530072147
H	29.74944086708973	-22.51586003238919	4.20254002827388
H	31.02219369871176	-21.79606222580779	5.19587066456904
H	29.89089589549761	-22.94619246082391	5.91105791204029
H	31.28169849467772	-24.04008273681939	1.37177735919236
H	30.19362467547726	-25.32739170754808	1.89576308743267
H	29.85964821804945	-23.65039497547113	2.34630813641587
H	33.82082715791869	-27.21988061110032	-0.18794672975202
H	34.37940340320957	-28.88695137765561	-0.37021680504864
H	32.80156004700318	-28.55561859879469	0.35520531617955
H	36.13408526564831	-29.94180000393603	0.35719286427836
H	37.48458177749594	-29.56455277442938	1.43252104850485
H	36.34048309399176	-30.83720194323496	1.86723139327584
H	33.38198506816043	-22.78769377027403	10.74428955878667
H	31.97626121479745	-23.13388869574471	9.72973257712051
H	33.19576411618867	-21.98239056971761	9.18117211603900
H	36.51971504850400	-24.53182424456019	10.86265811416640
H	35.37487980830771	-25.74684401698824	11.43460082262302
H	39.47608886449921	-29.27665753020060	8.84484240136529
H	39.11542748344431	-27.60556110838118	9.29762773861044
H	38.05225975903902	-28.91119278689494	9.82648676998445
H	38.59963336684578	-30.95940477749522	5.78478966194075
H	39.63626905675213	-29.63977500347382	5.23763243517962
H	39.75682632032814	-30.22541425852771	6.90139542712438
H	34.97280307570148	-24.02957377884823	11.55670051814381
H	36.27481588084182	-31.32114507807054	7.27896523091943
H	35.56729424044106	-32.88473633513578	6.80636293176264
H	35.57904871217929	-31.52128449226586	5.66667260202492
H	33.30585591246266	-31.77253084923124	6.63762208592643
H	33.97587241278151	-31.64150819481695	8.28257530063165
H	31.89838683562295	-26.53370509981405	7.13008860197310
H	31.22155019689043	-27.99718514841747	6.40033528364393

H	32.06391027532974	-28.10102478366875	7.94518401815216
H	32.43084567495115	-26.38128641204412	1.70958316822305
H	36.75021229282063	-26.72679354560586	9.55826997462472
H	37.44891852870069	-29.61175285317439	3.92249470217356
H	32.03500935263452	-23.16016296956417	7.19059010603281
S	36.07826219058729	-24.72827571946150	4.90476261520288
C	37.50546183527506	-25.42209358910807	3.98539558625357
H	38.11512447517057	-26.08037788259632	4.61517221533805
H	37.18184558453727	-25.99280656678415	3.10757014423137
H	38.13878962042340	-24.59533923937899	3.64171830673583

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B3LYP Scan/Thiolate IPC Model/BSS/110 degrees Constrained Optimization

C	30.64638611511296	-24.39842659828769	2.22079595000682
C	35.46291692559393	-24.77770119098269	10.91172112308296
C	39.05273036674805	-30.00909937610711	6.08607363610544
C	33.84756491016240	-28.19546849416130	0.29199265030655
N	33.08172969731602	-25.41944811274082	4.89021537355737
N	34.45599583330426	-25.52942458793303	7.37462726761131
N	34.84554564835447	-27.44616143654484	3.83209341642354
C	32.96788095225300	-26.40436911452423	2.65245966645072
C	32.64463732339866	-23.98191272540906	6.81970606769724
C	36.24389165816581	-26.67359379473162	8.59714546795957
C	36.78407995519491	-28.85445155073625	4.31815624042425
C	30.45192498277385	-22.74376301602706	5.01447159471867
C	33.06605390259848	-22.93630161405441	9.70717782973496
C	38.66263395235254	-28.56461003269194	8.97919954134897
C	36.43940860156645	-29.81816022629359	1.39634137058768
C	32.53822500458101	-25.52679233288258	3.64231947430257
C	33.60242239207165	-24.50857535724358	7.68210357060732
C	36.71308859864811	-27.50486424204438	7.58488972481107
C	35.78428251255179	-28.37337127916149	3.48047979946348
C	31.45858144488065	-24.56324809894108	3.47132471616774
C	33.82220984204175	-24.05100436468397	9.04637482281083
C	37.85298241852838	-28.40015327079323	7.72642845311820
C	35.58742651937811	-28.80723952275696	2.10488480561093
C	31.37677492845457	-23.86551899223331	4.64527929283687
C	34.82983668074176	-24.82579358103852	9.55283456051728
C	38.02055184482367	-29.00652658480800	6.51011370702191
C	34.49620145925361	-28.12650097265493	1.64220959526373
C	32.40134478683417	-24.41696037300046	5.52045377698435
C	35.21729458498719	-25.74139410141107	8.48838380602996
C	36.97453322204971	-28.48075806607368	5.64525792879908
C	34.04705608996607	-27.27788756891858	2.73817711075268
N	36.20400060556391	-27.57620185774657	6.31915417346227
Fe	34.61042579318817	-26.53834973021052	5.61775122764984
C	34.00440862810758	-31.38834744329292	7.18067384614738
C	35.43176006604789	-31.80029451918701	6.84885671994551
C	32.11126726477907	-27.60747037670243	6.99030404146848
C	33.38162678150832	-27.87495537229062	6.22642534876116
C	33.59006442691111	-29.32429116113280	6.03311472360479
O	33.51374380991518	-29.94791943666526	4.99582812578137
O	33.85326564697068	-29.96163318691127	7.23121232234499
H	29.72849196194896	-22.53842891325517	4.21746354114708
H	30.99959445220756	-21.81045694482286	5.20684973338148
H	29.87943231543406	-22.96958191527042	5.92495500522077
H	31.26023664920385	-24.04884278860852	1.37855685388590
H	30.18403765387592	-25.34441520777666	1.90658880103862
H	29.83968861082797	-23.67020736722909	2.35967689582934
H	33.81319094347275	-27.21074600821143	-0.19446858405829
H	34.38831684478961	-28.87197654622311	-0.37881591418718
H	32.81157518503127	-28.55674613390687	0.35604845526672
H	36.14827849797131	-29.92306339951924	0.34535962358393
H	37.50225617259468	-29.54042435192471	1.41464863954966
H	36.36042105877777	-30.81218803997976	1.85858235600001
H	33.39512746468425	-22.78471628768904	10.74112446030945
H	31.98529065449565	-23.13459939904564	9.73357259400443
H	33.20139393223084	-21.98336707814876	9.17692217638586

H	36.53181139329311	-24.52927714720941	10.85355759755784
H	35.38894072040119	-25.74369405760181	11.43073577094592
H	39.47497870154931	-29.28629601179417	8.83995634999110
H	39.11693029863428	-27.61608953614037	9.29779955272261
H	38.04900098893543	-28.92096604427458	9.81843391309617
H	38.59630224411475	-30.96273125635776	5.78589553341494
H	39.63680535123412	-29.65114428442348	5.22699395956869
H	39.76029421537981	-30.22685546579586	6.89394860416371
H	34.98673172616884	-24.02636536525586	11.55115605485498
H	36.13756093903029	-31.34907178930879	7.55020182311983
H	35.53502267468343	-32.89106550714223	6.89790496541571
H	35.69509117735886	-31.46952121455960	5.84340327855006
H	33.30622872702258	-31.79742731335248	6.44644913422657
H	33.71734889529387	-31.73370708676392	8.17802591689903
H	31.93900240352375	-26.54799978065889	7.16282451327019
H	31.23712332160730	-28.00595500101170	6.44930189606598
H	32.13096668816834	-28.11954114714580	7.96341646716659
H	32.43206837062701	-26.37867371237558	1.70824893347305
H	36.75637184511888	-26.72905285531345	9.55302597441461
H	37.46943340807121	-29.58840311226801	3.90508192844840
H	32.03249577677190	-23.16746424554723	7.19524326626515
S	36.07921597939998	-24.71002937590175	4.90753996080278
C	37.49980505316688	-25.39289435924833	3.97001501400091
H	38.11469108502475	-26.05682192521022	4.58861879619990
H	37.16959730603885	-25.95535950475607	3.08938635904217
H	38.12957881915332	-24.56216895496014	3.62947133468559

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B3LYP Scan/Thiolate IPC Model/BSS/120 degrees Constrained Optimization

C	30.63742391413367	-24.40152348092355	2.21815067630158
C	35.45622492482526	-24.82225981258483	10.90525714035961
C	39.07686149440195	-29.99337293361490	6.03974518231519
C	33.86985599214547	-28.15546766096668	0.25515567822703
N	33.08544394203900	-25.42155424028158	4.87584363083600
N	34.45625898251632	-25.54678374597351	7.36054279757187
N	34.85611131925582	-27.43487584320984	3.80442995422970
C	32.97289864365310	-26.39441494681456	2.63276142279262
C	32.64477962329787	-23.99672207293096	6.81443771677309
C	36.24416555121669	-26.69801382353539	8.57725516552123
C	36.80244533055595	-28.83651763643932	4.27935566546258
C	30.44260481082955	-22.76004595288321	5.02014467704967
C	33.06019675997635	-22.97333728570456	9.71083530151567
C	38.67521653503255	-28.57641447166969	8.94447751518243
C	36.47233068322786	-29.76940364329576	1.34790120186166
C	32.53991016183411	-25.52534089917397	3.6285698984816
C	33.60201141986009	-24.52843246654879	7.67413620415516
C	36.71817848280898	-27.51927123322137	7.55882657930658
C	35.80177622355261	-28.35202032029903	3.44534478698486
C	31.45505914501107	-24.56643037821307	3.46507466202358
C	33.81893089221316	-24.08161281072577	9.04227223054038
C	37.86389632810139	-28.40806043861791	7.69324315745358
C	35.61053201077538	-28.77307384718410	2.06516990607928
C	31.37301901345858	-23.87431933938911	4.64239812951527
C	34.82578036722853	-24.86005430255300	9.54481903948375
C	38.03608325581091	-29.00302716947952	6.47187649494129
C	34.51463019062382	-28.09631977955197	1.60768149242690
C	32.40206262621440	-24.42503957937557	5.51265016192494
C	35.21582564071967	-25.76711832193656	8.47407739725378
C	36.98720842178987	-28.47695875819837	5.61082867420633
C	34.05785818521307	-27.26176059055060	2.71146558465697
N	36.20995860195086	-27.58324066951102	6.29224210635325
Fe	34.61562094345926	-26.54138467086116	5.59587557591224
C	33.89101023512455	-31.39352297722644	7.24505135113010
C	35.35183224053429	-31.78766626323578	7.07534571366219
C	32.14090943603309	-27.60377961813590	7.01114860766261
C	33.38348844851083	-27.88726381188205	6.20720052352886
C	33.60865520046117	-29.33517720063243	6.04404896844082
O	33.66917600915610	-29.96773174163488	5.01081071463134

O	33.71684369691366	-29.97017674439407	7.27185241089427
H	29.71885641348795	-22.55144976161437	4.22430337080684
H	30.98582459680038	-21.82593311853445	5.22091255216584
H	29.87040276025832	-22.99619272234927	5.92821355724073
H	31.24753895053027	-24.05144197845891	1.37345249210758
H	30.17430155602689	-25.34774587403335	1.90571239054388
H	29.83085688028428	-23.67390634691441	2.36070778441602
H	33.83112195444858	-27.16613962425653	-0.22155441327393
H	34.41650459798152	-28.82197726589916	-0.42088551566567
H	32.83580980739521	-28.52347276390980	0.31233949319974
H	36.18354041102750	-29.86678767933393	0.29554484889694
H	37.53256655675295	-29.48215200152478	1.37040706755915
H	36.40166943168870	-30.76828756184971	1.80076577006157
H	33.38596386076353	-22.83101645004753	10.74714746239413
H	31.97955963851440	-23.17279252731444	9.73216240968726
H	33.19639195728094	-22.01547768296202	9.18979132660512
H	36.52519380283623	-24.57322405210871	10.85092815409137
H	35.38150538108992	-25.79213623873774	11.41687229908810
H	39.49343843641395	-29.29016425095644	8.79899935361873
H	39.12192852001430	-27.62686803207341	9.27067734619788
H	38.06503031866454	-28.94461961162310	9.78112251998128
H	38.62943423990955	-30.94802409358930	5.72949387986440
H	39.65897922473988	-29.62191861561269	5.18506623979720
H	39.78517589286780	-30.21290460054300	6.84643652992878
H	34.97882162706154	-24.07583225885178	11.54949452151856
H	35.97140747453360	-31.31683061730657	7.84266000033072
H	35.46578089329946	-32.87586028442474	7.15058684850002
H	35.71827362757017	-31.46568775485803	6.09985557246273
H	33.28404800303804	-31.81587104509452	6.44044036387277
H	33.49977107844524	-31.73962651241051	8.20618740107714
H	31.88462405999383	-26.54746651304448	7.02214069420283
H	31.27152584497719	-28.16094276014347	6.62679136814008
H	32.27978686698226	-27.93331879441299	8.05100408407942
H	32.43602012955244	-26.36555432664545	1.68924813950785
H	36.75572504314166	-26.75920805692060	9.53326656013848
H	37.49235101278608	-29.56246642164229	3.85989663759132
H	32.03079627736061	-23.18605046125759	7.19501110044335
S	36.07791354078163	-24.70725937371618	4.90180154336883
C	37.50449013693120	-25.37403596078488	3.96214389610146
H	38.12042291749523	-26.04112379611301	4.57625785141632
H	37.18015324049973	-25.92943386783016	3.07486743070234
H	38.13090403630446	-24.53658695693481	3.63213937421654

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B3LYP Scan/Thiolate IPC Model/BSS/130 degrees Constrained Optimization

C	30.64199284304489	-24.37444599751418	2.20089266591227
C	35.42064747641127	-24.92232603713292	10.90166678667947
C	39.09588240760913	-29.98488042418192	5.95656347825967
C	33.87657948669895	-28.10506932077076	0.19958546669364
N	33.08898240590447	-25.42226752547839	4.84865159729322
N	34.46089575519631	-25.57004125729336	7.33165609293545
N	34.85741743089805	-27.42440394898754	3.75857210124634
C	32.97289360766717	-26.37490531322264	2.59704579255911
C	32.64404690364441	-24.02044103729596	6.80341884901132
C	36.24280626373852	-26.74104554409169	8.53926326950648
C	36.81656772623586	-28.81549644700086	4.21234105532982
C	30.44801584550432	-22.75985031546962	5.01873213701576
C	33.02665503122773	-23.05945610041769	9.72509362448804
C	38.68240845353883	-28.61572678035640	8.88236062247674
C	36.48843875730024	-29.71715398975304	1.27213043477413
C	32.54267681717069	-25.51372406239328	3.60069142525611
C	33.59796230698496	-24.56389367196000	7.65911031695653
C	36.72451832555107	-27.54379519822182	7.50931952879677
C	35.80977404452499	-28.33024965067175	3.38739435025600
C	31.45894005700697	-24.55227316860753	3.44649090495963
C	33.80009506577285	-24.14630804062492	9.03844698627663
C	37.87368123228310	-28.42979365419829	7.63209462488317
C	35.62002558722195	-28.73617982643890	2.00261524520450

C	31.37738442139860	-23.87136382704282	4.63041486178170
C	34.80628651389520	-24.93082444205002	9.53349882261089
C	38.04996508856079	-29.00584177786519	6.40227695606918
C	34.51928179000662	-28.06120597169908	1.55377096628556
C	32.40564143807021	-24.43140418051719	5.49552021056465
C	35.21183789676368	-25.81159853260584	8.44682629613947
C	36.99980197453080	-28.47216222822489	5.54774696651264
C	34.05863341020700	-27.24203263814344	2.66746344556546
N	36.21829220668680	-27.59153499602528	6.24112832597979
Fe	34.62162089013827	-26.54459857743069	5.55759172798440
C	33.82069187801569	-31.36241262492080	7.39486565579286
C	35.30097538785346	-31.71455896087112	7.45421491398060
C	32.16535390697576	-27.58642187905632	7.01138812101539
C	33.39592839742120	-27.89940912439963	6.19786786638946
C	33.66627743061670	-29.34188881135239	6.10762178495669
O	33.89039521375644	-30.00384707872198	5.11537924373099
O	33.60753568223363	-29.94602439465334	7.35926043770287
H	29.72426512859605	-22.54339472739188	4.22502404443683
H	30.99220526880087	-21.82817495947032	5.22789981438757
H	29.87591521212178	-23.00390381341694	5.92474098593955
H	31.25258840794666	-24.01529176636674	1.36036000658405
H	30.17948250817398	-25.31749305427877	1.87815299377492
H	29.83500174083974	-23.64874433631723	2.35049610105741
H	33.84322407192185	-27.11115999413979	-0.26805695099576
H	34.42160338228717	-28.76761207073963	-0.48163479081638
H	32.84070254744262	-28.46875504895140	0.25096871623624
H	36.19681824711869	-29.80645256113347	0.21982527949488
H	37.54600302568099	-29.42015450839157	1.29373028396024
H	36.42875872495352	-30.72101686433885	1.71523801404554
H	33.33662465471342	-22.94329368041676	10.76946276646799
H	31.94699235300132	-23.26478326339690	9.72544806010841
H	33.16521474723688	-22.08731870354621	9.23186578747264
H	36.48961798973097	-24.67002785603361	10.86571353810961
H	35.34180706657099	-25.90354408971448	11.39056590050489
H	39.50188046901251	-29.32615935172885	8.72805701273116
H	39.12703069046680	-27.67066300187129	9.22398415813582
H	38.07079380203724	-28.99752196714081	9.71190857290441
H	38.65264698846653	-30.93272259127323	5.62088577654088
H	39.68422762561971	-29.59320677798634	5.11521132359595
H	39.79777703431399	-30.22169520539266	6.76385551387373
H	34.93407373380609	-24.19144971035869	11.55673548764346
H	35.78187776415958	-31.22540316721648	8.30516253600642
H	35.43383452440300	-32.79873959876061	7.55335126531315
H	35.80300031826464	-31.38375874570297	6.54441364605240
H	33.35357019370011	-31.82027727195758	6.51942429772803
H	33.29987916945110	-31.70130020386668	8.29530478288051
H	31.76944771195862	-26.59855624577555	6.78483408013664
H	31.36311024868717	-28.32431596908518	6.86773326705809
H	32.40955549528724	-27.60025928487302	8.08352976767974
H	32.43575613126971	-26.33696274243471	1.65402509975782
H	36.74909893805178	-26.81774856220578	9.49693337051811
H	37.50901573299057	-29.53343731404334	3.78362326245904
H	32.02589748332235	-23.21788560080035	7.19419340598345
S	36.07820785577685	-24.70549175932742	4.87968402982043
C	37.51672517015406	-25.35790586692019	3.94858282953463
H	38.13017545318335	-26.02640574437182	4.56362508623223
H	37.20347627795945	-25.90855200038337	3.05434900502324
H	38.14179543725102	-24.51488276081463	3.63053231778871

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B3LYP Scan/Thiolate IPC Model/BSS/140 degrees Constrained Optimization

C	30.61742079127275	-24.41318701544102	2.21879864508476
C	35.44622972833681	-24.91157766515618	10.89418451171404
C	39.12406796139466	-29.96280629722140	5.94196697644541
C	33.88450881802678	-28.10736867401931	0.19890404135535
N	33.09298239187819	-25.43104542164681	4.85115501755069
N	34.47335481128966	-25.57095059073680	7.32974268864153
N	34.87552238073614	-27.41362622576507	3.75247424769717

C	32.97097366960927	-26.38887234698377	2.60205172896949
C	32.65337678551897	-24.02412793801742	6.80372906662040
C	36.25605048166755	-26.74173988127107	8.53615040105236
C	36.85006685197599	-28.78525236899061	4.19732557521257
C	30.43417528493847	-22.78738282601054	5.03141727107401
C	33.05270051910109	-23.04786104458881	9.71822088168089
C	38.69399744459210	-28.61879712511427	8.87694236724057
C	36.52585402759129	-29.68142810003537	1.25645215113073
C	32.53836276425730	-25.53093039906953	3.60747493758678
C	33.61290945532244	-24.56232919038269	7.65653823435693
C	36.73953288081690	-27.54081831017994	7.50404898062339
C	35.83850049052515	-28.30574755182300	3.37564224302821
C	31.44600595654007	-24.57874118110189	3.45839056620944
C	33.82059699790698	-24.13980623328826	9.03339226454468
C	37.88995921347838	-28.42519833464673	7.62489160162789
C	35.64811687602887	-28.71213151686077	1.99134963450880
C	31.36903566911084	-23.89321801618128	4.64010145260636
C	34.82636973645273	-24.92501070575128	9.52846830539135
C	38.07320567332670	-28.99053376095390	6.39105184235564
C	34.53484488969479	-28.05346888755991	1.54907253092678
C	32.40763579462936	-24.44237585458625	5.49955363315492
C	35.22679329517713	-25.81032358156941	8.44375322655104
C	37.02509033037129	-28.45323241927990	5.53636935131612
C	34.06872596680010	-27.24147955019342	2.66584193632755
N	36.23711134546073	-27.58188988182345	6.23390261283625
Fe	34.63608109894419	-26.54234486292070	5.55367651446524
C	33.69421368162872	-31.41650596659783	7.31302371112457
C	35.16463207919760	-31.72139196745526	7.57040892676562
C	32.20329262755127	-27.58673981238313	7.04253458747841
C	33.40792914136806	-27.91256285434456	6.19652366019283
C	33.66720997518932	-29.35310606292159	6.08353546613198
O	34.02353036030446	-29.98446718653468	5.10910939882312
C	33.43924223091596	-30.00814139126108	7.29388540728254
H	29.70572025718682	-22.57627379695730	4.24058770623972
H	30.97332952133126	-21.85210036618786	5.23741455210109
H	29.86747913580241	-23.03421659899843	5.94006793521357
H	31.21930671428413	-24.05837282963140	1.37021501283934
H	30.15554219624405	-25.36035938006019	1.90737614429702
H	29.80914782669730	-23.68928465881943	2.37007001027803
H	33.83080439789915	-27.11390596386818	-0.26770278441879
H	34.43686439242513	-28.75978406455297	-0.48620336596726
H	32.85548930844150	-28.48925354316730	0.25636125966688
H	36.22985469646925	-29.77530426385616	0.20577602100499
H	37.57939954254352	-29.37014694141213	1.27254186442771
H	36.48196106064158	-30.68566767667194	1.70053553569635
H	33.36962272152384	-22.92550748752391	10.75979155044169
H	31.97280324298120	-23.25186589777488	9.72692989262005
H	33.18926171824805	-22.07909414579282	9.21791145644924
H	36.51527827493660	-24.66045472249388	10.85279145209136
H	35.36852023300388	-25.89065341461183	11.38751268157321
H	39.51623166579813	-29.32555145704395	8.72053648716706
H	39.13452005711574	-27.67516420839063	9.22776628238566
H	38.08010463897928	-29.00885776539189	9.70088676110455
H	38.68450488577324	-30.90685236351231	5.5913677756926
H	39.71865094177140	-29.56026184115458	5.11014275444009
H	39.81977002724916	-30.20838024198144	6.75199184469233
H	34.96300022572642	-24.17755988380314	11.54821812759234
H	35.49990007989123	-31.25153324247243	8.49890330274500
H	35.32594920567244	-32.80327812895827	7.64946868493116
H	35.77763440973566	-31.33639360658270	6.75443644561547
H	33.37241436409680	-31.85701549002867	6.36634887035711
H	33.06561267726632	-31.80543653283758	8.11969560713041
H	31.80367752252623	-26.60076822789019	6.81406055908410
H	31.39705861895440	-28.32518055208399	6.93687095755557
H	32.47985104888120	-27.58339579895156	8.10684658024262
H	32.42736145464203	-26.35822180627166	1.66250146959404
H	36.76215632828173	-26.81990625224035	9.49380876321611
H	37.54847881147676	-29.49545112953871	3.76546374028735

H	32.03503671358641	-23.22189036862874	7.19478474216007
S	36.08135580098024	-24.69306397110057	4.88602181382776
C	37.50893139278458	-25.32907900302306	3.92751824654810
H	38.13022090516816	-26.00596310938413	4.52520648655241
H	37.18550948161780	-25.86688719358875	3.02914886205609
H	38.12895970743465	-24.48042317209077	3.61468571690486

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B3LYP Scan/Thiolate IPC Model/BSS/150 degrees Constrained Optimization

C	30.59804661386705	-24.41867939953199	2.22630497275428
C	35.44437028259613	-24.99492289229507	10.88451890575859
C	39.16781805140459	-29.92916282998804	5.84352321281751
C	33.86270362461941	-28.09160192362666	0.16372128357614
N	33.09937697601258	-25.43779741310033	4.83356936349360
N	34.49171206771053	-25.59304325135259	7.30436535056420
N	34.88516970804207	-27.39998537759352	3.70903316921435
C	32.95656122899695	-26.39202033005487	2.58393825565226
C	32.66874655352949	-24.04323228159670	6.79682357024105
C	36.27406933034845	-26.77843467329104	8.49628237388777
C	36.89253518316639	-28.73293039263635	4.12021222265566
C	30.44127275245528	-22.79534989236086	5.04255092460909
C	33.05538668533561	-23.11322441108572	9.72764937971569
C	38.71800591598832	-28.65408935825851	8.80798514682193
C	36.54964373998632	-29.61712645263350	1.17734170232991
C	32.53261191309949	-25.53641508868359	3.59525752640182
C	33.62752280813517	-24.59163935595209	7.64373934860293
C	36.76633042239968	-27.55282334009461	7.44937461465665
C	35.86249216157942	-28.26845746020195	3.31371374235184
C	31.43824874245971	-24.58503840469381	3.45794681344827
C	33.82907356220491	-24.19161755394552	9.02799874957097
C	37.92082721412336	-28.43446595990441	7.55597087295729
C	35.66237478447710	-28.66984386868819	1.92949696171489
C	31.37273757776775	-23.90042733472264	4.64106911758986
C	34.83300562602265	-24.98447636777849	9.51501593555295
C	38.11307950752209	-28.96942259609482	6.30998550900121
C	34.52960626224008	-28.03174164324870	1.50566531438331
C	32.41876423956946	-24.45089308645949	5.49013311133087
C	35.24092384908025	-25.84988053918418	8.41734588096818
C	37.06521588252752	-28.41941159415271	5.46321458953327
C	34.06308240782757	-27.23414202631058	2.63240918857541
N	36.26949994582458	-27.56879617186286	6.17656556413962
Fe	34.65615245497547	-26.54218712656040	5.51971686004644
C	33.61064738454203	-31.41321924896619	7.39184298102573
C	34.96885733815380	-31.64507653820368	8.04256375608679
C	32.19822920477214	-27.60010151816953	6.96146739634833
C	33.44365640569050	-27.93024970172610	6.17960842638134
C	33.75608365859565	-29.36255466287148	6.14313200858668
O	34.32304898782331	-29.99169868886461	5.27194172288582
O	33.30880560158425	-30.01907564065702	7.29507954917585
H	29.71036634998400	-22.57825865876696	4.25564984860337
H	30.98312391164350	-21.86248332750087	5.25211055204727
H	29.87738816982720	-23.04654806240624	5.95178724751799
H	31.19317434189568	-24.06886012982010	1.37095025192819
H	30.12864707449806	-25.36446085122351	1.92176830839020
H	29.79453833380016	-23.69078300116090	2.38361015153385
H	33.78562706430935	-27.09734070678372	-0.29781346359903
H	34.41759487626092	-28.73123169442592	-0.53134039859544
H	32.84117939739568	-28.49143004605538	0.23244896087327
H	36.23237593487063	-29.72317934680786	0.13407472352773
H	37.59436942718852	-29.27692721799470	1.16870672238241
H	36.54384323175891	-30.62039558605164	1.62565848143166
H	33.36831050603929	-23.00662277266005	10.77214191855863
H	31.97615772303929	-23.32079212839793	9.72929616171226
H	33.19059228041579	-22.13615648830727	9.24341505834620
H	36.51399982739429	-24.74472285814252	10.85411658179154
H	35.36210906259025	-25.98200412738089	11.36093697592474
H	39.54378519681528	-29.35420513877987	8.64052775902238
H	39.15304423325267	-27.71732780547682	9.18326968093730

H	38.10009229131326	-29.06525605733857	9.61847577236625
H	38.72960654939048	-30.86558130432704	5.47173734216909
H	39.76362555289491	-29.50758359745106	5.02208144615921
H	39.86185158896095	-30.19045902405329	6.65005783498341
H	34.95806728319231	-24.27129570761785	11.54778256589493
H	35.01189171099970	-31.16291572537085	9.02330904894541
H	35.15728760432287	-32.71741980158779	8.17395070850509
H	35.76429785124623	-31.22767364466453	7.42257678695296
H	33.58116415222146	-31.86144035053502	6.39635646134671
H	32.80764768778485	-31.83980793295053	8.00106077893374
H	31.79860495697604	-26.62432606204605	6.69528409768540
H	31.40822957400325	-28.35165423940149	6.83519934539277
H	32.42423748756541	-27.57424342459755	8.03747304984250
H	32.40214627160995	-26.36283877453155	1.65065940257352
H	36.77620238992194	-26.87384776936866	9.45445112308616
H	37.59972479223557	-29.42655704016113	3.67595196547106
H	32.05059807895490	-23.24538850428751	7.19701865802875
S	36.06987243714833	-24.66928550531286	4.84736791981979
C	37.54011750620234	-25.28227057618451	3.94042750555779
H	38.15691352240664	-25.93998797018957	4.56366511257908
H	37.25768066191343	-25.83546960293363	3.03745027076824
H	38.15110313369743	-24.42299113954211	3.63898631119541

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B3LYP Scan/Thiolate IPC Model/BSS/160 degrees Constrained Optimization

C	30.56452891813704	-24.50108984430635	2.26580582050714
C	35.49517455852293	-24.93409240106179	10.88347517198943
C	39.25279234935448	-29.84222554201655	5.84534876055033
C	33.86668291100847	-28.13891523843350	0.20318007574809
N	33.10829788212718	-25.45563464861489	4.85631172885881
N	34.52390473274104	-25.57057938757892	7.31522882471060
N	34.91119184847088	-27.40191443941309	3.73307547701204
C	32.95078806753608	-26.44098424149703	2.62118720505559
C	32.68788478663367	-24.03694374180749	6.80446554448451
C	36.32220064249557	-26.73280095527111	8.50529403774058
C	36.95376943813744	-28.68442512634900	4.13041635418040
C	30.43011490271923	-22.83300643959742	5.05691292207177
C	33.09057907810541	-23.07462367349780	9.72352910458507
C	38.79087247702601	-28.57688784313239	8.81219292467960
C	36.60345417138461	-29.58903338862152	1.19345426220489
C	32.52713438274043	-25.57864446433647	3.62685671460610
C	33.65658078945697	-24.57021965426046	7.65014411712771
C	36.81920726047442	-27.50454654387313	7.45868735463105
C	35.90561674394571	-28.248343856466975	3.33153056790221
C	31.42189673172199	-24.64010800662383	3.48907754829640
C	33.86472542362221	-24.15607957793458	9.02914577205403
C	37.98796817535322	-28.36816133310778	7.56202428045691
C	35.70080718887792	-28.66101258499321	1.95147843537566
C	31.36593122179385	-23.93664514596513	4.66169571532478
C	34.87514845164004	-24.93979446297088	9.51781321278542
C	38.18589878379414	-28.89809758400537	6.31528294090260
C	34.54722746041158	-28.05411467444540	1.53704740964318
C	32.42721216469500	-24.46450403895543	5.50607837902950
C	35.28123097996902	-25.81296687517365	8.42590776281769
C	37.12602544018520	-28.36620483992936	5.47208909065465
C	34.07424212504794	-27.26113599240187	2.66417796668452
N	36.31818836033195	-27.52979407981788	6.18816923477879
Fe	34.68681635123786	-26.53320882287273	5.53827622093077
C	33.36415141944396	-31.49279986830419	7.20548614166135
C	34.64184069619130	-31.84969670340721	7.95609796067392
C	32.24785635283643	-27.59300722552700	7.00792952218648
C	33.48787513523909	-27.93267031648596	6.22302122359575
C	33.77903856734041	-29.36770711636703	6.16391229917604
O	34.47766594575706	-29.96642840882110	5.36839550300714
O	33.13341752257456	-30.08283418794656	7.18242070808875
H	29.68465040873433	-22.63814879127776	4.27784859989930
H	30.96605431494176	-21.89115948744202	5.23983514909913
H	29.88329036161354	-23.07201804492339	5.97969575418881

H	31.14456927454060	-24.15532443119934	1.39850015552919
H	30.10368931636366	-25.45676197106737	1.97974705896404
H	29.75377362212180	-23.78130469304485	2.42341641637338
H	33.74104071110509	-27.14759358845041	-0.25362981022550
H	34.44000289472284	-28.75192787505972	-0.50094176522114
H	32.86415256864725	-28.58271651723583	0.28268155997081
H	36.28023579733282	-29.70384005837458	0.15291975850057
H	37.63987775451604	-29.22470894236325	1.17617179344697
H	36.62465585695055	-30.59166181776648	1.64282136570066
H	33.40758910828055	-22.95891536003207	10.76582498125213
H	32.01204961381961	-23.28564497999808	9.73137765541056
H	33.22063687818232	-22.10092003222020	9.23115426455932
H	36.56230667321368	-24.67453371025150	10.84448323011426
H	35.42488754224609	-25.91825051798983	11.36778229144430
H	39.62246207311082	-29.26998152622962	8.64412680606551
H	39.21866591756819	-27.63526622443623	9.18379479448405
H	38.17894620811798	-28.99124767146357	9.62561381326513
H	38.82556329529822	-30.78226627877054	5.47001366566603
H	39.84327335246842	-29.41003364597814	5.02548081291014
H	39.95018486400019	-30.09805065425899	6.65077289090162
H	35.00647165984825	-24.20990998420614	11.54434929288066
H	34.61646247854743	-31.44865340186791	8.97354942522930
H	34.76285325555500	-32.93801374581722	8.01594881383231
H	35.51009711787316	-31.43326208830086	7.44307989867556
H	33.40763178630925	-31.87126193036902	6.18141090316788
H	32.48740307355906	-31.91620250312912	7.70535016456654
H	31.89079498576377	-26.58927763948884	6.79477812230822
H	31.43169998777449	-28.30419899355368	6.82933590872653
H	32.45838499789525	-27.64157861265064	8.08666999912418
H	32.38504892822347	-26.43138951689533	1.69433011998253
H	36.82976601424570	-26.81867456008958	9.46152362656967
H	37.67367708976364	-29.36281157263254	3.68302858048441
H	32.06817043398071	-23.23817507705795	7.20030142167636
S	36.07107201217468	-24.64417111909390	4.84741554274379
C	37.52837281747715	-25.23444072955706	3.90521882875741
H	38.16489249535243	-25.89040855862187	4.51024007592952
H	37.23267315477050	-25.78437302109474	3.00444249571811
H	38.12351554890731	-24.36631694954459	3.59762564646742

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B3LYP Scan/Thiolate IPC Model/BSS/170 degrees Constrained Optimization

C	30.53703362123495	-24.57053580084750	2.31492473978606
C	35.55617972793382	-24.86470814956200	10.88691892761847
C	39.33284621992766	-29.75789967054043	5.85381094915629
C	33.83803843810873	-28.22373534667048	0.26978134860120
N	33.11665046764991	-25.47205542790369	4.88891122225367
N	34.55396999376104	-25.55158619652585	7.33633183976285
N	34.93580342561891	-27.40177284141213	3.76412811064871
C	32.93974659232180	-26.49232379218732	2.67139530218860
C	32.71090020983404	-24.02749310930253	6.82108780071258
C	36.37032591516188	-26.68790737978884	8.52192137663356
C	37.01107423146561	-28.63536360763008	4.14651684469385
C	30.43101115378887	-22.85702203436474	5.07951694293305
C	33.14128549154938	-23.02197536198075	9.72230926541199
C	38.85784769319716	-28.50470448199615	8.82349356572525
C	36.62721934555889	-29.59304257822384	1.22817749693997
C	32.52107477939906	-25.61793344065067	3.66887988251428
C	33.68816187548914	-24.54759482239612	7.66551740655237
C	36.87113532144925	-27.45586087363073	7.47431816402370
C	35.94211817289225	-28.23174935777551	3.35751178448698
C	31.40974177647277	-24.68678825372978	3.52973553195157
C	33.90810622794262	-24.11430965781532	9.03684318412809
C	38.05287568614684	-28.30217777338210	7.57364072871692
C	35.72098798293499	-28.66985940453106	1.98786064356800
C	31.3655527369475	-23.96422738215358	4.69133644174634
C	34.92326736466570	-24.89069524453836	9.52734876411266
C	38.25654096384850	-28.82584731860123	6.32561409777980
C	34.54574476398794	-28.09606002102614	1.58612791917264

C	32.43847447443152	-24.47462240464422	5.53150952168727
C	35.32157813147895	-25.77714590531338	8.44330427731374
C	37.18599923078405	-28.30993732980945	5.48592283591189
C	34.07691258749390	-27.29432425451275	2.70856858426447
N	36.36681300321879	-27.48766957140523	6.20566758662449
Fe	34.71714780619585	-26.52266121267911	5.56269932704789
C	33.18419712493816	-31.55809198385236	6.94009666076830
C	34.32814825477703	-31.99362352495391	7.84913046316211
C	32.27405012808675	-27.61637184334257	7.00944245847625
C	33.52917098992273	-27.94221425682595	6.24421695652575
C	33.80530094012850	-29.37790024452365	6.14649095532866
O	34.63768114454410	-29.94392316687905	5.46189784728988
O	32.97463526221722	-30.14583765171045	6.97703225769319
H	29.68275616040806	-22.66928938869651	4.30138670985741
H	30.96785683408726	-21.91366580140923	5.25156090537640
H	29.88729980573290	-23.08702115998957	6.00649857158098
H	31.10796795520081	-24.25025028578867	1.43201322266814
H	30.06491163010874	-25.52906556557586	2.05794913568480
H	29.73397887680996	-23.84076082571723	2.46584298091801
H	33.65814549886196	-27.24364718753231	-0.19281792518586
H	34.42045924242049	-28.81868404759489	-0.44238191033733
H	32.85793749258169	-28.70979770346094	0.37784592746464
H	36.29010779500264	-29.72667208813553	0.19427771254631
H	37.65728703214052	-29.21267779185462	1.19061327068109
H	36.67123566485045	-30.58932296166946	1.68997167634563
H	33.46950979221162	-22.88974452970870	10.75917522993427
H	32.06275145487754	-23.23203497616016	9.74494774771840
H	33.26665424118345	-22.05634154895684	9.21304273706211
H	36.62172420795383	-24.60093699234230	10.83462855371736
H	35.49485105907029	-25.84288769168748	11.38438404042753
H	39.69698718621955	-29.18837825586512	8.65435405166703
H	39.27517426575455	-27.55943456872322	9.19788446137066
H	38.24983330915743	-28.92746578795265	9.63560944121515
H	38.91453849627526	-30.70388492101461	5.48329355376915
H	39.91474862628297	-29.32125760024797	5.03017756323413
H	40.03656159679561	-30.00320804004881	6.65704965136080
H	35.07034926216603	-24.13431542572618	11.54310292431288
H	34.15722215177230	-31.65616432901725	8.87569688703057
H	34.41959119862194	-33.08645649302929	7.85636569612438
H	35.27002037406584	-31.57007819003510	7.49762836229875
H	33.37895347600794	-31.87066783120541	5.91113231381021
H	32.23604947796166	-31.99309654709316	7.27095611913106
H	32.02276123134112	-26.56144893056615	6.96524137586012
H	31.41462031615169	-28.19432835167557	6.64311001161495
H	32.38355673250536	-27.89494594820872	8.06760916823366
H	32.35978854713701	-26.50532677774917	1.75335607626506
H	36.88494424807655	-26.76368236062655	9.47526176567047
H	37.74057533133063	-29.30155444056373	3.69629896046194
H	32.09315471847287	-23.22442182965363	7.21131584192934
S	36.06328251045815	-24.61719851697083	4.85055335916084
C	37.51555384285810	-25.18593550465071	3.88815956654213
H	38.16893396586873	-25.83430786557333	4.48315140531314
H	37.21506211204633	-25.73823254286700	2.99036646609050
H	38.09443716991614	-24.30913581503631	3.57416078315984

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B3LYP Scan/Thiolate IPC Model/BSS/180 degrees Constrained Optimization

C	30.64344869791828	-24.63413305553279	2.36119573939435
C	35.96226453486240	-24.88974870047264	10.75275512078140
C	39.39669292135406	-30.00704497997665	5.71068673784721
C	33.78026759339362	-28.40246449440779	0.26803873496101
N	33.29568945344015	-25.54674023624682	4.85634427742884
N	34.80489622747588	-25.62823470584882	7.25990024287548
N	34.98471234040039	-27.59003750693015	3.72900013060518
C	33.00280861635058	-26.61432987809235	2.67158272237485
C	32.98799261468047	-24.06016929805450	6.77763221686347
C	36.61467444493901	-26.80738759208744	8.41440641463489
C	37.04012958536011	-28.86561460316143	4.06724952773228

C	30.67630301525901	-22.86701604310491	5.09373787693703
C	33.56590231839407	-22.99327185504866	9.63052334557416
C	39.05767787321627	-28.68764815743400	8.67051763659725
C	36.54927499584214	-29.84705137128144	1.17143589060459
C	32.64930511507104	-25.70360943119287	3.66276565967488
C	33.98306849460627	-24.58780384953059	7.59624888290244
C	37.04487110702100	-27.62356620754165	7.37287950948359
C	35.95567689178215	-28.45031124177565	3.30573569742878
C	31.55844718259565	-24.74720036374767	3.54497674882670
C	34.26948096517469	-24.12859910965229	8.94653200084359
C	38.21103147076983	-28.49494762634050	7.44726070782627
C	35.68723644818473	-28.89480623856017	1.94622708460436
C	31.57280727330602	-24.00145311810174	4.69356722216421
C	35.27586286893337	-24.92821678211887	9.41925548156008
C	38.35551714976497	-29.04756013782001	6.20465575462793
C	34.52148292554119	-28.28861276049499	1.56690788369080
C	32.66245911580214	-24.52160238041961	5.50482430527931
C	35.60119201747367	-25.85605555619195	8.34629097545502
C	37.26398149067120	-28.52645686477245	5.39533157453912
C	34.10684257315739	-27.46071130652355	2.69241260764171
N	36.48867752854355	-27.67642193154110	6.12775983629767
Fe	34.86244078074541	-26.65296209082875	5.51178999458092
C	32.87702704070129	-31.59915701627208	6.68252818858169
C	33.81912063498320	-32.18628720909440	7.72781397746708
C	32.41970943332455	-27.60376669600326	7.05679496856700
C	33.62646321787982	-28.00218212001019	6.24965639997180
C	33.79496658715500	-29.45179847788768	6.11318659908893
O	34.66815525000039	-30.06146390885365	5.52367414286723
C	32.79109644372611	-30.17736791558717	6.77539007139504
H	29.91151826702072	-22.67106911337752	4.33412131094797
H	31.23900860887850	-21.93414454472927	5.23902178573220
H	30.15310488277292	-23.07267443656682	6.03804037988062
H	31.18731741524622	-24.34580564467435	1.45061535820394
H	30.14073665676128	-25.58640934175271	2.14265860703028
H	29.86290389610303	-23.88323781683644	2.52610371846843
H	33.63345988629472	-27.42130825034369	-0.20398177780004
H	34.32121376511568	-29.03077621432169	-0.44801429238291
H	32.78237470765431	-28.84372778644995	0.40296123159862
H	36.17573485566791	-29.98850609824930	0.15115428370508
H	37.58447903779688	-29.48727661548345	1.09457986410735
H	36.58931990234732	-30.83747170841908	1.64599675918929
H	33.96764064506619	-22.81790947471122	10.63458745546018
H	32.48858432284096	-23.18387669354442	9.73758402628604
H	33.66779872789295	-22.05467683544347	9.06815028623382
H	37.03990484302415	-24.70189749754876	10.64909176785176
H	35.85736916207631	-25.84053482788688	11.29401013327276
H	39.88015563401417	-29.38672367504603	8.48364030627301
H	39.50246450371826	-27.74240569472008	9.01197773908637
H	38.47371257046955	-29.08669930062162	9.51201394733210
H	38.94851709198734	-30.95178199846605	5.37316372989474
H	39.95428604405104	-29.59424620789306	4.85862027651179
H	40.12553778106560	-30.25010426047621	6.49188369772517
H	35.55210100543740	-24.10201878547204	11.39428088333193
H	33.52281532821252	-31.87450182563104	8.73382720166909
H	33.80520116541211	-33.28212945458042	7.68883748191288
H	34.84027540244242	-31.84764866200695	7.54634745250647
H	33.20382507511770	-31.88063784500092	5.67835317354220
H	31.85379767275986	-31.95551885728352	6.83664619019245
H	32.26307520786882	-26.53017782518380	7.06887412806225
H	31.50750317747071	-28.08559811743277	6.68096770830283
H	32.51923683842790	-27.94289407156705	8.09864304569279
H	32.39453306683124	-26.62184757912289	1.77193182160803
H	37.16259648107545	-26.87458243444227	9.34962836829352
H	37.74281291642247	-29.55013083573771	3.60225315639625
H	32.40382646187778	-23.23508988458801	7.17373698726744
S	36.44331356387413	-25.03746648992851	4.59325022792714
C	35.91701119230575	-23.32949802147349	5.00167218802366
H	34.92682866145743	-23.10120221675072	4.59118330295382

H 35.88346191376399	-23.16276040402268	6.08450725375600
H 36.63847310657551	-22.62649993366983	4.56832034937452

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B3LYP Scan/Thiolate IPC Model/BSS/190 degrees Constrained Optimization

C 30.60330332081050	-24.74667489759886	2.44079450492038
C 36.06257112383543	-24.77926200993338	10.74684577975987
C 39.49019411108082	-29.93040938316345	5.73516246264992
C 33.76221342708556	-28.50106056651820	0.35891215154240
N 33.30510103171623	-25.57967473076453	4.91075018752748
N 34.86076764257811	-25.59301874305618	7.28606847776256
N 35.00996187820559	-27.61525514472136	3.78671385788648
C 32.99686660359968	-26.68544256558848	2.74637666270068
C 33.00422437743359	-24.06837931639672	6.81253920375959
C 36.70830878622247	-26.72309977430567	8.42864796131928
C 37.09051311021486	-28.85272355586932	4.11246984101178
C 30.64575005594751	-22.94016613695592	5.14710109221210
C 33.61371967508678	-22.94332161472348	9.63664916988769
C 39.17811566596975	-28.56763147583769	8.67812078814435
C 36.56526460988921	-29.89138496522061	1.24006872276442
C 32.64384190138077	-25.76527542432532	3.72915596666344
C 34.02504750649633	-24.56256892167757	7.62037723873188
C 37.13289890079292	-27.55031094222953	7.39379532503710
C 35.98627137586946	-28.46884574687925	3.36200497852065
C 31.53579709275612	-24.82880386364893	3.61357196173381
C 34.32608983092328	-24.07672335051141	8.95849171198115
C 38.31217182612057	-28.40436755757724	7.46416025184737
C 35.70210744183314	-28.93976425410358	2.01453795966930
C 31.55403890094178	-24.06671326766833	4.75151130198234
C 35.35493434806605	-24.85033466074773	9.42588309698654
C 38.44497085209190	-28.97522929814477	6.22889464354523
C 34.52203145558065	-28.35557808495212	1.64398151118773
C 32.66406349905779	-24.55658559506170	5.55372058111934
C 35.67871746142433	-25.78918605016903	8.36198590216546
C 37.33311186602995	-28.48326712306480	5.42887059954433
C 34.11359033841183	-27.51517422001807	2.76217811527494
N 36.55791863518586	-27.63138886558537	6.15923619326598
Fe 34.90362499253229	-26.64677800001641	5.55515568667091
C 32.71307650079961	-31.56902181269959	6.29342213334675
C 33.37205141229515	-32.28384689433753	7.46810359332945
C 32.45510130681429	-27.61398326018432	7.08325609866827
C 33.68879036910301	-28.00296149988734	6.31162176453888
C 33.82905445922304	-29.44800481136429	6.11362392638116
O 34.78503773980197	-30.06637779814807	5.68380351742054
O 32.67213591147510	-30.15443910293400	6.48012962661041
H 29.87073412414043	-22.76401973160255	4.39297866957194
H 31.19702777003053	-21.99804920071992	5.27526122733078
H 30.13476849799887	-23.14131682541361	6.09904181345978
H 31.13381223809248	-24.48142835487611	1.51552730014377
H 30.09798462780764	-25.70430551751118	2.25345238159532
H 29.82468784848382	-23.99206047666921	2.59755639207269
H 33.59439710681007	-27.52994633760371	-0.12667379805575
H 34.30082659799566	-29.13352772345384	-0.35524171414657
H 32.77278662294147	-28.95361241612600	0.51654201307346
H 36.17157767896396	-30.06128926902554	0.23172185062175
H 37.59121182351044	-29.51349849001933	1.13185751664032
H 36.63575201261403	-30.87081016169587	1.73341804179520
H 34.02337805921393	-22.75077465395964	10.63435214514474
H 32.54036633347851	-23.14757331003982	9.75713929165922
H 33.69668200802863	-22.00999214860747	9.06247727229012
H 37.13242601389670	-24.56111463212027	10.62335612355681
H 35.99441454070070	-25.72776551267985	11.29776595866244
H 40.00392556487644	-29.26288632074265	8.49169366198584
H 39.61924394913502	-27.61281961058751	8.99701232766428
H 38.60948967839661	-28.95708058913258	9.53446712805306
H 39.04753438922542	-30.88426867925357	5.41664622126730
H 40.03297055470011	-29.52398005224934	4.87050188748146
H 40.23114659119953	-30.15505615537977	6.51048442408930

H 35.64008387344224	-23.99807773842871	11.38833533935149
H 32.86684260422895	-32.03438001545157	8.40601734701719
H 33.32910182408931	-33.37124325656450	7.33295147229699
H 34.41929086399340	-31.98815890253697	7.54731561278870
H 33.24287270012840	-31.79944567995283	5.36567788605080
H 31.66641700429466	-31.87183826480236	6.19185208652255
H 32.45255868948503	-26.56487304966607	7.36247994582125
H 31.55411919297265	-27.80197610856465	6.48076762987380
H 32.33199555340751	-28.21893936797974	7.99084401478075
H 32.37487067124060	-26.71609917542682	1.85661905081906
H 37.27197884040565	-26.76721076832836	9.35584353484567
H 37.79535269453172	-29.53542947318169	3.64802660417330
H 32.41155197344955	-23.24820425187071	7.20622743115974
S 36.44125105583458	-25.02169839212801	4.58161233247596
C 35.88937213270923	-23.31662167069657	4.96800378339369
H 34.88535633433888	-23.11655840485515	4.57687653590248
H 35.87819880763538	-23.12807570300345	6.04777486173200
H 36.58577420688734	-22.60823532050168	4.50345884496539

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B3LYP Scan/Thiolate IPC Model/BSS/200 degrees Constrained Optimization

C 30.57350143265779	-24.83189610238465	2.50031066100060
C 36.14779664778270	-24.67202652509320	10.73052376341046
C 39.54855956768470	-29.88453682703818	5.76598695188587
C 33.74272518881978	-28.58709600679580	0.43612158162690
N 33.30852483303850	-25.60604892871869	4.95293924985769
N 34.89403737939192	-25.56836857049153	7.30840711863272
N 35.02633052941112	-27.63732977341252	3.83326096840843
C 32.99272961852117	-26.73945888510411	2.80374381463433
C 33.00723449861078	-24.07911431445639	6.84183272507702
C 36.77757811868260	-26.65099048186066	8.43774073894486
C 37.11741211958198	-28.85730303716287	4.15685050737568
C 30.61784436012669	-22.99870327682771	5.18826512184294
C 33.64683768577184	-22.89840422369806	9.63689901512754
C 39.26687896794726	-28.46720609009213	8.68586974226211
C 36.56274563065693	-29.94910518810986	1.30750325263307
C 32.63871142610632	-25.81222167531374	3.77964105537199
C 34.04715158299647	-24.54619300266151	7.64105631308415
C 37.19532628423549	-27.49183745766342	7.41155800290753
C 36.00205979348333	-28.49308597907213	3.41199824265218
C 31.51750780955076	-24.89125822636630	3.66528361104427
C 34.36379231455042	-24.03300939922596	8.96542882717720
C 38.38305239677371	-28.33424700869969	7.48107604679327
C 35.70432607687958	-28.98840675102192	2.07614444671365
C 31.53612967367175	-24.11822129787385	4.79580464021120
C 35.41448366715164	-24.78083772873744	9.42617117814114
C 38.50280309750696	-28.92783746429215	6.25549159054759
C 34.51723752167690	-28.41564579412145	1.70924416676905
C 32.65993698178723	-24.58576253267768	5.59233317712290
C 35.73400466510080	-25.73271131611360	8.37245752041190
C 37.37551121384902	-28.46010192503005	5.46212966102924
C 34.11701640313471	-27.55897639892889	2.81778708316567
N 36.60375571642219	-27.60063476022854	6.18707882424216
Fe 34.92952955240079	-26.64539214210154	5.59110564000592
C 32.63769987909320	-31.51098615859375	5.95342767923537
C 33.01068814720405	-32.33762852541415	7.17882758509450
C 32.50841092356562	-27.63633238061845	7.14821149842219
C 33.73762727012806	-28.00767464036879	6.35997622335737
C 33.85918145355713	-29.44630352158664	6.10641101391844
O 34.85047336006258	-30.08531940751604	5.80944938442936
O 32.63050176617725	-30.11117762744852	6.23587154118779
H 29.83386498205698	-22.83953768597300	4.43963154114389
H 31.15896662597055	-22.04881019705460	5.30159948504156
H 30.11810630677542	-23.19589736047257	6.14697050499098
H 31.09307524777686	-24.57265150351836	1.56719143090702
H 30.07548456223076	-25.79629264190041	2.32881987200807
H 29.78936715035944	-24.08266042262626	2.65535931404799
H 33.56600524699090	-27.62563606340193	-0.06528175842755

H	34.27480019595544	-29.23117866005374	-0.27251248091062
H	32.75667617416060	-29.03941981898575	0.61402169534435
H	36.15615013273509	-30.13993844124010	0.30803568682130
H	37.58474926290978	-29.56729108833062	1.17796472614945
H	36.64626051180379	-30.91878676166180	1.81774174034716
H	34.06968864838473	-22.68477398474952	10.62478630377825
H	32.57833221224194	-23.11459292898448	9.77771164000769
H	33.70843663610150	-21.97326815781352	9.04698206098430
H	37.20866736250968	-24.42770105514706	10.58099574252807
H	36.11653054941583	-25.61356121576184	11.29646646557888
H	40.09414766309339	-29.16145663223793	8.50230455565670
H	39.70654441798025	-27.50346421498047	8.97894294881052
H	38.71248348886171	-28.84212875470540	9.55783902420924
H	39.10798003217634	-30.84535415363729	5.46622234991885
H	40.08125514764309	-29.48849226538463	4.89025733221122
H	40.29787703794129	-30.09367217262062	6.53762922232476
H	35.71832546223818	-23.89270527944348	11.36963843102461
H	32.34397155835200	-32.11113406747774	8.01629433519659
H	32.93577571601114	-33.40959113548953	6.96011706094143
H	34.03614695291984	-32.11956897114512	7.48188364127577
H	33.33186006653000	-31.71264851623508	5.13420958547963
H	31.61973507097020	-31.74091352505454	5.62450565427143
H	32.53494842712746	-26.60810887544660	7.49788069557560
H	31.61027049436763	-27.75462652112507	6.52471349895668
H	32.35632392037419	-28.29648082033287	8.01259532919772
H	32.36125406604737	-26.78796948126157	1.92148710734972
H	37.35668374219542	-26.67142852026301	9.35623323005704
H	37.82058748226644	-29.54463156652048	3.69672220552225
H	32.40740757918248	-23.26291783127215	7.23305170033337
S	36.43194714166022	-25.01472233210819	4.57428009146841
C	35.87761574004199	-23.31214364202508	4.96736167568776
H	34.86327261367470	-23.12084698106688	4.59893249677011
H	35.89000856156387	-23.12009093561452	6.04647782861320
H	36.55824525264886	-22.60079046395293	4.48443286305031

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B3LYP Scan/Thiolate IPC Model/BSS/210 degrees Constrained Optimization

C	30.56683313697962	-24.87666279126611	2.49301945955477
C	36.14843469773418	-24.62594804401829	10.71690928083082
C	39.55984648263559	-29.87402851769518	5.79621983193734
C	33.75624156710711	-28.62633980236298	0.45106100499105
N	33.30592777867280	-25.62224248309670	4.94972034744098
N	34.89147965376633	-25.55952727487655	7.30530107806851
N	35.02819695255425	-27.65753520335254	3.84757065381272
C	32.99631529308746	-26.76878450831682	2.80716427745014
C	32.99620326629936	-24.08546332966607	6.83078870843354
C	36.78211246845344	-26.62409122446418	8.44150572981863
C	37.12098168003041	-28.87200177833920	4.18212636141018
C	30.60017635269561	-23.02885448995154	5.17076887104815
C	33.63095557742249	-22.88103933828540	9.61685177279277
C	39.28271073274166	-28.42440853684387	8.70030512193504
C	36.57670282166820	-29.97846525617890	1.33699957723150
C	32.63770114950051	-25.83779482777047	3.77722306848374
C	34.03920129497809	-24.54040814846639	7.63200986118045
C	37.20133839524845	-27.47373612363924	7.42308719613167
C	36.00639575271128	-28.51373481005377	3.43309143240762
C	31.51191835666059	-24.92351379008458	3.65766828923007
C	34.35380842815550	-24.01582803906821	8.95212428718086
C	38.39265110097654	-28.31039554628580	7.49804496139556
C	35.71351379789890	-29.01665838992545	2.09889092538070
C	31.52527557377810	-24.14479588405374	4.78421341166250
C	35.41062771031812	-24.75273187504067	9.41666181658892
C	38.51043484245140	-28.91781534896318	6.27893451720909
C	34.52662267086597	-28.44784870840129	1.72571711653992
C	32.65144030235725	-24.60202332955751	5.58393365993373
C	35.73416049489655	-25.71075727716832	8.36936652835351
C	37.37888053012797	-28.46343348219813	5.48380638543634
C	34.12201960703617	-27.58602923181653	2.82885015343001

N	36.60665586058711	-27.59806210749388	6.20148672392089
Fe	34.92890326737051	-26.65195310539780	5.59770101332540
C	32.54072415489613	-31.44102910596083	5.77636942056154
C	32.85360932482876	-32.35611760063055	6.95488878471120
C	32.67492337994948	-27.62398095634881	7.38252765188657
C	33.75841447723521	-28.00637908529561	6.40819058541801
C	33.82626599823940	-29.43620668668967	6.09283199207007
O	34.80272103434660	-30.09313980890539	5.78687134940449
O	32.57205833296709	-30.06196334702766	6.14698865570429
H	29.81421845540348	-22.87958791158392	4.42216100371824
H	31.13518912970090	-22.07472325266541	5.27750125234784
H	30.10286891153540	-23.22321484037990	6.13131933044557
H	31.08484042654758	-24.62335551422700	1.55745491265407
H	30.07194288876098	-25.84413482748790	2.33006996412536
H	29.7804450531118	-24.12871903560604	2.64269907905991
H	33.58113648688687	-27.66761116254550	-0.05611746854956
H	34.29067961932270	-29.27422306420610	-0.25232674216481
H	32.76965982920305	-29.07774484260294	0.62822032163359
H	36.17275550459327	-30.17577935473512	0.33771868275413
H	37.59756589229416	-29.59359164592007	1.20738788138276
H	36.66276136970759	-30.94517686805379	1.85237655105504
H	34.04639165159390	-22.66586684743516	10.60756636034527
H	32.56177779617817	-23.09843376255262	9.75016811809775
H	33.69571426710661	-21.95633394463373	9.02653841891775
H	37.20040870298106	-24.34798525503230	10.56217799946805
H	36.14995875836672	-25.56986802318258	11.27951774408403
H	40.11166448643236	-29.11792307033993	8.52162832295248
H	39.72011717559960	-27.45530006983680	8.97866732759406
H	38.73421593399324	-28.79006637381499	9.57990109616827
H	39.12404203979481	-30.84066940833910	5.50840328281674
H	40.08704651676793	-29.48441774993223	4.91430520375087
H	40.31331074579552	-30.07032370135436	6.56723918286450
H	35.69907496097074	-23.86259697379687	11.36158959157583
H	32.17473178961566	-32.15879692290206	7.79002334533619
H	32.74594142954480	-33.40854982427538	6.66629314838895
H	33.87831614554469	-32.19510539680788	7.29367513547019
H	33.24889831802123	-31.61406290376859	4.96266798673256
H	31.52466911829801	-31.61338936454145	5.40898526453847
H	32.29731805565274	-26.61875766344472	7.20234789128718
H	31.83618170833192	-28.32460541084924	7.37934007009419
H	33.08762320613366	-27.61535303866821	8.40393798023351
H	32.36672900067236	-26.82406396203708	1.92398953220702
H	37.36327623355922	-26.63283259998411	9.35891305954175
H	37.82571028331518	-29.56144007398269	3.72754581875569
H	32.39135342865568	-23.27030581966437	7.21645948091697
S	36.42002702518202	-25.02635017487159	4.55366979596297
C	35.90133181552802	-23.32452337612034	4.99528224928137
H	34.88453185037433	-23.10834377805115	4.64765860284615
H	35.93369641303094	-23.15811834835203	6.07810399485067
H	36.58597828346112	-22.61330164645663	4.51786436215517

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B3LYP Scan/Thiolate IPC Model/BSS/220 degrees Constrained Optimization

C	30.52465763055005	-24.98540793532433	2.54959889293110
C	36.22129247375493	-24.50923206522123	10.68658674271697
C	39.59096216644556	-29.85966510539538	5.84352572241175
C	33.74611172660201	-28.71285375217039	0.51872483435466
N	33.29903426906208	-25.66013900531917	4.98697596674019
N	34.91786582404647	-25.53478609982431	7.31841687706159
N	35.03878758649493	-27.68757481368414	3.89088646313446
C	32.98825955111585	-26.83290392023277	2.85842008398798
C	32.98684042261375	-24.10542061412069	6.85228343772238
C	36.84151942493811	-26.55039404145453	8.44381646893770
C	37.13755219572943	-28.89024307102387	4.23084409940573
C	30.55199801350405	-23.11119998862817	5.20869248335445
C	33.65009982357318	-22.83587190180059	9.60284552657691
C	39.34745219430410	-28.34114542209017	8.71449072419476
C	36.57930386615797	-30.03924101395910	1.40424277262832

C	32.62348210945390	-25.89898283288002	3.82316709398966
C	34.05188185579595	-24.52633859867659	7.64272762478123
C	37.25108590610914	-27.42063707239776	7.43927857098077
C	36.01773032578981	-28.54544478648108	3.48229968151098
C	31.48103085812515	-25.00530937012329	3.70580240532429
C	34.38059206062344	-23.97074720704805	8.94656035439403
C	38.44407453580097	-28.25449973438867	7.51979569382505
C	35.71698942672280	-29.07027211724694	2.15815475945388
C	31.49131040765406	-24.21611041814874	4.82489825017824
C	35.46018397018211	-24.67824646358586	9.40460947449778
C	38.54739049967814	-28.89136388645765	6.31460264908546
C	34.52471279486022	-28.51218401735202	1.78516243820060
C	32.63358257107060	-24.64569891937344	5.61755462059803
C	35.78145253455300	-25.65088040495467	8.36986953638469
C	37.40670322290543	-28.45546921316368	5.52159739638275
C	34.12357651998091	-27.63679333510418	2.87868215814123
N	36.64194871120622	-27.57401241615197	6.22797936310077
Fe	34.94640125134963	-26.65488381669761	5.62741264945099
C	32.46360014271362	-31.29467781314777	5.46110112826477
C	32.57502658932319	-32.31269185197639	6.59020591275086
C	32.77627766748044	-27.66051365777938	7.50048059652596
C	33.81080763549068	-28.00658517315700	6.46056604165206
C	33.83535933702496	-29.42058523830271	6.07272149724247
O	34.80096482111739	-30.12369140822433	5.85117538096202
C	32.54741542271525	-29.95032639017261	5.93932367532117
H	29.75425672793098	-22.98530552697644	4.46825949985650
H	31.07183022602215	-22.14670930995367	5.29606337261399
H	30.07031395723045	-23.30125887693730	6.17800433186655
H	31.03236493169965	-24.74489857264588	1.60512807451386
H	30.03492326046835	-25.95887660171796	2.40800824128171
H	29.73472818828219	-24.24010448751995	2.69364330413981
H	33.56265271615528	-27.76241171817547	-0.00087112880024
H	34.27882200372046	-29.36826903498341	-0.17898544825490
H	32.76312298171832	-29.16651626233411	0.70943496479049
H	36.16869625727031	-30.25376455304166	0.41123516791406
H	37.59714029780046	-29.65129025965275	1.26097755896900
H	36.67433482066377	-30.99755799973794	1.93351956121706
H	34.07182959468556	-22.60271151597190	10.58684189169149
H	32.58491949943975	-23.06417941124780	9.74874282376370
H	33.69854151312743	-21.91824026504126	8.99998004927167
H	37.25654225896589	-24.18696950067310	10.50623433275562
H	36.27645996158281	-25.44730955021718	11.25606133652773
H	40.17276446076303	-29.04089675553442	8.54351569251779
H	39.79019376998394	-27.36669689958210	8.96438682427351
H	38.80818916294320	-28.68391664610652	9.60886102380947
H	39.14962422495920	-30.82859268072845	5.57255774646272
H	40.11744243500162	-29.48678562336144	4.95391755878305
H	40.34589251156832	-30.04743963854067	6.61527159749482
H	35.75383429013321	-23.76067185184590	11.33576254354760
H	31.82417347981825	-32.11938125622496	7.36241354227298
H	32.42199789868108	-33.32968424079392	6.20980238641458
H	33.56496247573245	-32.26093516748484	7.04642132257474
H	33.24621350941560	-31.46425471911765	4.71772701652352
H	31.48726481315926	-31.35994134706417	4.97208389628949
H	32.33891260632682	-26.67536971539424	7.33404025078516
H	31.96962472567532	-28.39698935723671	7.55869184834643
H	33.25472560230786	-27.61551997059328	8.49101345171193
H	32.35112823045728	-26.90644422453247	1.98203692732289
H	37.43655628544541	-26.53406186161851	9.35220783236501
H	37.83906345347193	-29.58805759033501	3.78416537624609
H	32.37243750386043	-23.29588876395828	7.23486690772646
S	36.38229683318979	-25.03064874462461	4.51166305448496
C	35.93473200813255	-23.33410606067276	5.04413489651238
H	34.89812792752702	-23.08883895124017	4.78618186327229
H	36.05706444342159	-23.20261349608895	6.12532056864088
H	36.59346480464106	-22.62014309725052	4.53531488834453

B3LYP Scan/Thiolate IPC Model/BSS/230 degrees Constrained Optimization

C	30.50239628129606	-25.03005607937902	2.60323916205574
C	36.27536679079851	-24.44306585598498	10.68019205575757
C	39.60022412652673	-29.86100211726966	5.87871033816351
C	33.69855126234187	-28.79031254249801	0.59631081397362
N	33.29806876564184	-25.67234444420934	5.02541817775017
N	34.93645737889854	-25.51815768834443	7.34136538051910
N	35.02574300129813	-27.72109986052019	3.94131358463979
C	32.97035707944808	-26.87130916899304	2.91356397209060
C	32.99313674758052	-24.10393059426776	6.88000378779391
C	36.88397674768201	-26.50393557732102	8.45255009858073
C	37.12270014878853	-28.92641645695626	4.28243807530123
C	30.54303261760057	-23.13174345760905	5.24474977562218
C	33.67626370702547	-22.80373755023691	9.61185794178881
C	39.39920562046984	-28.28225268857133	8.71971443387037
C	36.53104297609428	-30.12093604695943	1.47864120376739
C	32.61403418074108	-25.92518241558782	3.86953880996572
C	34.06720582210220	-24.51220705120089	7.66486415411596
C	37.28453332916485	-27.38734944992707	7.45605304491496
C	35.99624676458787	-28.59160794734364	3.53830827164791
C	31.46789254733635	-25.03579820175595	3.75201709011992
C	34.40759674897752	-23.93990145529454	8.95872365724917
C	38.47916686029114	-28.21925899269433	7.53630671547411
C	35.67993317238597	-29.13683277736395	2.22608493700988
C	31.48344767176531	-24.23672401343229	4.86384518908773
C	35.49903831296442	-24.63303195801683	9.41028177750270
C	38.56436575037561	-28.88164563924786	6.34383630928456
C	34.48813509732401	-28.57586815325172	1.85382944967625
C	32.63343464111571	-24.65529502980323	5.65181713915114
C	35.81502270691414	-25.61477581341291	8.38233645266662
C	37.41220700829155	-28.46134234436131	5.55843130665038
C	34.10177442362713	-27.68058714270454	2.93603593942371
N	36.65930153978057	-27.56317030008614	6.25637486041624
Fe	34.95300129104182	-26.65778092307727	5.66487253785262
C	32.59589745504658	-31.20013998944081	5.18763055127553
C	32.43048677655450	-32.26026344804711	6.26956635987490
C	32.75808651022468	-27.66898362618189	7.51419747164139
C	33.83412241766951	-27.99356037821043	6.51058966547585
C	33.88609435658941	-29.41068496548072	6.12672599578980
O	34.84894523256823	-30.14887148295798	6.09868807794915
C	32.63375998373012	-29.87662822412900	5.73055885744254
H	29.73754355955387	-23.01744320138572	4.51084106343111
H	31.05936192871495	-22.16406800291733	5.31653838968807
H	30.07171971309830	-23.31328886956426	6.22076903566173
H	31.00193775378820	-24.79809790269599	1.65230129306510
H	30.01385579672302	-26.00605353302998	2.47557715985804
H	29.71187412056624	-24.28509302390692	2.74589174099221
H	33.51987593781253	-27.84684502036508	0.06254294464235
H	34.22028606042912	-29.46182649169887	-0.09434173934013
H	32.71284219484459	-29.23160705267713	0.80136861491086
H	36.10667358882475	-30.35320399074936	0.49545612931283
H	37.54710776337355	-29.73672350972468	1.31426002588139
H	36.63318943483802	-31.06956106242061	2.02381496440512
H	34.10660787533542	-22.55861754226965	10.58921308305502
H	32.61421278084445	-23.03773755862665	9.77088315534332
H	33.71228020823281	-21.89146014423648	9.00005035868423
H	37.30373510285067	-24.10884227447715	10.48297167502043
H	36.35065109303294	-25.37534891922707	11.25682409698945
H	40.22327500048519	-28.98385235966724	8.55034085344692
H	39.84351770765871	-27.30266882358087	8.94548687186950
H	38.87302735442941	-28.60940984912088	9.62760706121894
H	39.15506603667002	-30.83668253538756	5.64003364262199
H	40.11098080691311	-29.51045871127315	4.97105701456659
H	40.36857472549438	-30.02914153682735	6.64168139016832
H	35.80694745871261	-23.69502080846442	11.32928924665017
H	31.53552747127801	-32.06798342528902	6.86920374164159
C	32.33560237680615	-33.25637286474393	5.82103923342244
H	33.29887072708399	-32.26269993711193	6.93052346738420

H	33.50757496065059	-31.37869899129170	4.61345756972847
H	31.74092993220060	-31.20001599881843	4.50558526045450
H	32.33856522846854	-26.67389196393172	7.36427171648719
H	31.94085047612645	-28.39830238874126	7.50574393689255
H	33.18864388961828	-27.66910428486667	8.52806502521137
H	32.32570718300848	-26.95474056034328	2.04356867079987
H	37.49127356856970	-26.47076452190380	9.35233499187227
H	37.81612279799058	-29.63667423415939	3.84271196158682
H	32.37801413744202	-23.29394317913859	7.26053915349528
S	36.37265352140393	-25.04775854029075	4.50669735319776
C	35.90947470689750	-23.34498059023043	5.00544038136834
H	34.87052628237913	-23.11471948864078	4.74292893063775
H	36.03058438476987	-23.19121797122170	6.08383233365875
H	36.56116549941783	-22.63456348285111	4.48273177668378

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B3LYP Scan/Thiolate IPC Model/BSS/240 degrees Constrained Optimization

C	30.49105681727869	-24.98312747160783	2.65309887495238
C	36.36433358765240	-24.38468597315144	10.65724596909629
C	39.53326306147441	-29.93924425608811	5.90396944401777
C	33.60249514124447	-28.81725044069054	0.65924758385766
N	33.29134999637719	-25.65186257685466	5.06336281549010
N	34.96084902336774	-25.49252707935722	7.35581856347613
N	34.97995958416001	-27.73919356823158	3.98053973647603
C	32.93405959491765	-26.85807543241792	2.95997156170242
C	33.01660658702651	-24.07270438533820	6.91190781259203
C	36.92617440319326	-26.47063988878830	8.44139738128527
C	37.04823083568502	-28.99278553396799	4.32549972295481
C	30.56644853836065	-23.07977265343462	5.29089102508331
C	33.74583189700196	-22.75462762238035	9.62330622628335
C	39.41852306014801	-28.27931985274106	8.70264934153457
C	36.40282841477445	-30.21401548238683	1.54268687327848
C	32.59795458794012	-25.90060968401653	3.91218230965044
C	34.09930813144041	-24.48176324531963	7.68515162219441
C	37.29785135268904	-27.37693752091239	7.45469334746823
C	35.92331576519521	-28.64278325616969	3.58457916215197
C	31.46164971202490	-24.99751742062806	3.79741636396697
C	34.46448107956989	-23.89732964375128	8.96740039413139
C	38.47888214483574	-28.22830603052667	7.53424424296958
C	35.58229987443984	-29.19877432104176	2.28301955214831
C	31.49196064766575	-24.19633407711652	4.90728546246134
C	35.56444150285951	-24.58605039907460	9.40384417753575
C	38.52777735268170	-28.92464715676267	6.35969112085866
C	34.40456891646176	-28.60862067660027	1.90993463256512
C	32.64208873968590	-24.62532324237652	5.68939343692662
C	35.85950561888218	-25.57888478943733	8.38028464207014
C	37.36969959821347	-28.50106968598095	5.58434528257687
C	34.04917444616984	-27.68949457481773	2.98228443161026
N	36.64781033030625	-27.56923679672831	6.27107157194550
Fe	34.94167214247449	-26.65298885238998	5.69492494289183
C	32.95039800533539	-31.23581870278674	5.07228136127039
C	32.47848113993941	-32.23271816042922	6.12313414671392
C	32.60798189960342	-27.67467286809969	7.37637767276486
C	33.82197838908729	-27.96725876793232	6.53526570415993
C	33.96321855185273	-29.40344169111353	6.23565966951758
O	34.88517827781645	-30.13690433891706	6.52253709427106
O	32.86501711277256	-29.88315554850918	5.53889001099463
H	29.75674848759319	-22.95946517351192	4.56262274306666
H	31.09366181385458	-22.11747246785768	5.35530014581470
H	30.10057541731364	-23.25270084595538	6.27109063008654
H	30.98909031904933	-24.76036030435278	1.69916401998638
H	29.98953146804343	-25.95322645936322	2.53035742468717
H	29.71052115044059	-24.22788032214578	2.79691148914154
H	33.45455274537348	-27.87759902020088	0.10946725285911
H	34.09745247259307	-29.51858308412198	-0.02139580078933
H	32.60270655846702	-29.21975432969390	0.87554326553372
H	35.95936074973133	-30.45674809840931	0.57053835653174
H	37.42365146400085	-29.85306996766296	1.35627446912506

H	36.49561627593152	-31.15426706084075	2.10403134255132
H	34.19180773211425	-22.50352889813885	10.59211488568738
H	32.68583463177571	-22.98494008002375	9.80019739951680
H	33.77449010519540	-21.84679927821939	9.00445373164874
H	37.38807423074917	-24.04995650964819	10.43805089806957
H	36.45227469957443	-25.31239440501391	11.23934123723329
H	40.23245692895332	-28.99252382299210	8.53261727726399
H	39.87645583358587	-27.30047312775892	8.90267574699130
H	38.90455278323170	-28.58451767969854	9.62505136508056
H	39.06562180862797	-30.91608814713063	5.71837148631044
H	40.02262724993392	-29.63441811462298	4.96853866243820
H	40.32092117393967	-30.08994742877712	6.65064093277460
H	35.90656030452987	-23.63251015978581	11.30921780848902
H	31.46326241756213	-31.99595232918025	6.45544256695401
H	32.47734904790547	-33.25017965909187	5.71436816805342
H	33.14274922225824	-32.21083397247033	6.98876478225747
H	33.97989295626905	-31.44814266905359	4.77734546368424
H	32.31257466449523	-31.26669865371660	4.18515608630166
H	32.53521012551795	-26.62653635083601	7.65755250934271
H	31.69262383417408	-27.94731683622221	6.83129461014291
H	32.60488840952654	-28.27466286208158	8.30068512200939
H	32.28260160449748	-26.93636290546354	2.09449604107892
H	37.55170416924427	-26.42678586740852	9.32812377298215
H	37.71838737388325	-29.72976796950650	3.89354787009108
H	32.41157296246448	-23.25655084251941	7.29538398764346
S	36.37203931218902	-25.06840307311686	4.50276101194041
C	35.87205876230080	-23.35303096494634	4.91692329592377
H	34.83444358268976	-23.15222874527138	4.62621033151398
H	35.97112219331063	-23.14914984927611	5.98938317788372
H	36.52115209450191	-22.65497499503728	4.37461614420157

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B3LYP Scan/Thiolate IPC Model/BSS/250 degrees Constrained Optimization

C	30.49062547499121	-24.95810548430264	2.65272926357138
C	36.36764696977676	-24.38905319171188	10.65665418532202
C	39.51359518735178	-29.95663240845367	5.90033337365608
C	33.57626647285750	-28.81386542735479	0.66358004535883
N	33.28931908966094	-25.63887603567370	5.06178125828161
N	34.96176546692972	-25.48545082367938	7.35247792704967
N	34.97222490715307	-27.72874514198885	3.97478968702994
C	32.93138381164894	-26.83664729978213	2.95411189165564
C	33.01053973679058	-24.07182559345695	6.91988195150355
C	36.93544968867067	-26.45878352330396	8.42746379522309
C	37.02238194959092	-29.01016325957032	4.32877295824520
C	30.55861803947685	-23.07376913294398	5.30463223156158
C	33.73539021628596	-22.76989627934710	9.64035995044968
C	39.42647574435088	-28.26959313737920	8.68363039366258
C	36.35610512339418	-30.24520035881498	1.55668216123147
C	32.59729201353844	-25.88081387921324	3.90850921027330
C	34.09560456673178	-24.48170838876198	7.68969377911734
C	37.30276002088527	-27.36709034520292	7.44115920921781
C	35.90090540564051	-28.65049939809084	3.58648252552524
C	31.46022546615873	-24.97794571584368	3.79780345081614
C	34.46058494187783	-23.90271580788907	8.97462305012026
C	38.48036531853003	-28.22317432079489	7.52032094279598
C	35.55057591377038	-29.21285215907501	2.28979907624550
C	31.48760708267957	-24.18475206243474	4.91334656383019
C	35.56646487751293	-24.58654319828866	9.40349201309439
C	38.51736781287227	-28.93144150391004	6.35255171743951
C	34.38181451868099	-28.60802014435107	1.91259355658655
C	32.63792832582475	-24.61705432508650	5.69355597815117
C	35.86445140615939	-25.57179987978270	8.37340819766847
C	37.35696908715213	-28.50787913173353	5.58051271425995
C	34.04010610831268	-27.67620385219385	2.97861804490666
N	36.64547780418066	-27.56457078197286	6.26232338380029
Fe	34.94026455952370	-26.64315184501041	5.68903112081492
C	33.17567673266283	-31.29047601036128	5.09329120543778
C	32.40701945814332	-32.18806550133444	6.05437007710434

C	32.60647135794446	-27.68261725503643	7.35600410468563
C	33.83507514308914	-27.95725597514408	6.53088142665148
C	34.02568359727056	-29.40232862885170	6.30099428814874
O	34.88845058493331	-30.11470987959303	6.76797744307920
O	33.05585876736697	-29.90846536342227	5.45618667067250
H	29.74882158446023	-22.95070499517679	4.57693023108132
H	31.08274415802655	-22.11032408661422	5.37649172870296
H	30.09288815321521	-23.25550976436284	6.28332303396398
H	30.98959064486879	-24.73118840458962	1.70028240608679
H	29.98897483259026	-25.92755358207085	2.52501498801128
H	29.71006056670514	-24.20339773004329	2.79922037884302
H	33.44254888219377	-27.87634162471517	0.10650751044537
H	34.06015076904770	-29.52796148587789	-0.01176791202853
H	32.57043669100224	-29.19909781880230	0.88313271522613
H	35.90818027065482	-30.48932275187715	0.58691587037641
H	37.38165905040554	-29.89997118842524	1.36634307500745
H	36.43667816966162	-31.18236289987416	2.12506473893007
H	34.18719367222632	-22.51675848886118	10.60593126317857
H	32.67953206905104	-23.01230242691294	9.82604713980709
H	33.74850021599899	-21.86005243896232	9.02404050928207
H	37.39123372078558	-24.05397838863833	10.43745899930934
H	36.45585469037831	-25.31859049645149	11.23583979965547
H	40.23900226712035	-28.98413100149825	8.51240771253553
H	39.88602375396939	-27.29015767824141	8.87665258935623
H	38.91724458299031	-28.57046122530344	9.61005897173025
H	39.03986901852949	-30.93379652594849	5.73211251471187
H	39.99539899724591	-29.66653466980988	4.95635705394002
H	40.30755870008236	-30.10141698917034	6.64142577953633
H	35.91060487445903	-23.63881567441981	11.31136053754746
H	31.35970941017665	-31.87893170666442	6.12084222813030
H	32.43589900153692	-33.23076147229195	5.71677482661553
H	32.84668966031074	-32.13925295021683	7.05280061861290
H	34.23191987098762	-31.56430453150809	5.07169263897360
H	32.76940125218754	-31.35366242956645	4.08081864071252
H	32.49389386470162	-26.62982922487160	7.60514984388855
H	31.70437166093822	-28.00292370585353	6.81288782812395
H	32.61926538845182	-28.25567918609982	8.29726271338864
H	32.27975199628799	-26.91175711180654	2.08846535904162
H	37.56490733489017	-26.41362511178436	9.31134407652869
H	37.68211029090850	-29.75902933301359	3.90105748237529
H	32.40270766123957	-23.26059318149952	7.30937933197325
S	36.37495723073007	-25.05765798091154	4.50379082503430
C	35.85809279561973	-23.34312472504554	4.90168475985495
H	34.82151555643329	-23.15231102485867	4.60075301987577
H	35.94670724222935	-23.13087011685607	5.97346343550458
H	36.50604569632807	-22.64348841936185	4.35998691188317

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B3LYP Scan/Thiolate IPC Model/BSS/260 degrees Constrained Optimization

C	30.48584975769879	-24.96486919590499	2.64417608819974
C	36.37248112836184	-24.36191371827501	10.63914560160716
C	39.49175764327638	-29.97819672801822	5.92053467360520
C	33.58391545705371	-28.81059848770922	0.65484485512355
N	33.27962084537494	-25.64553745615346	5.05859806250750
N	34.95472787854147	-25.48318515578680	7.34780942146946
N	34.96449909899319	-27.73521878967194	3.97571099815644
C	32.92974060121064	-26.83889453998658	2.94736119956681
C	32.99944569298813	-24.07595953682538	6.91472882610501
C	36.93155717003847	-26.44984246453708	8.42327562450721
C	37.00617193979128	-29.02774155730246	4.34080104224036
C	30.54445675739853	-23.08511349155723	5.29940137820498
C	33.73500415260632	-22.75319172633642	9.62232253521348
C	39.41604401068552	-28.26797755233016	8.68961622965257
C	36.35138121724471	-30.25634878542759	1.56401472760738
C	32.59071043895431	-25.88666354851912	3.90341453090120
C	34.08895141250894	-24.47820985812302	7.68216664795334
C	37.29435180370613	-27.36642491527276	7.44309163499939
C	35.89056527477216	-28.66149565560556	3.59257522634811

C	31.45219173134833	-24.98572875352167	3.79198456130685
C	34.45811281447881	-23.89029017897115	8.96167261080875
C	38.46815605995594	-28.22701889046277	7.52753228384983
C	35.54516212199045	-29.22198598996597	2.29357812115322
C	31.47556160988934	-24.19459976961201	4.90896512827485
C	35.56661300967311	-24.56984281206782	9.39066550568808
C	38.50037811281461	-28.94522064544351	6.36560668978624
C	34.38192587515148	-28.61098805729251	1.90969270355541
C	32.62564256670036	-24.62564646565612	5.69063230971236
C	35.86137959579139	-25.56182813944886	8.36597128967261
C	37.34166953035331	-28.52180398758436	5.59097415112498
C	34.03807394324158	-27.67868971924614	2.97486849509640
N	36.63487799724875	-27.57005144586746	6.26613412519209
Fe	34.92939404466026	-26.64824549007598	5.68759126209357
C	33.21165861757405	-31.27041747269925	5.03937801779406
C	32.37592304384016	-32.15462070837469	5.95576466539936
C	32.68340689488218	-27.69457366481499	7.47402019452569
C	33.83641363798677	-27.95756519323692	6.54281017806690
C	34.01424212124194	-29.40536584642477	6.30909007652947
O	34.82439634710153	-30.13607103533468	6.83880644375166
O	33.09839340523079	-29.88581298698487	5.39759276707927
H	29.73147304344993	-22.96769598177537	4.57431303757610
H	31.06561514600540	-22.11955546719188	5.36510830885739
H	30.08330283240236	-23.26431457662580	6.28067455531642
H	30.98558567562708	-24.72507738440922	1.69522832350682
H	29.99371539994177	-25.93775647337402	2.50654784712244
H	29.69802886080945	-24.21855193580726	2.79475702507786
H	33.46698410349149	-27.87329167978301	0.09355592550054
H	34.06390937540970	-29.53321725868519	-0.01419214295190
H	32.57140689267420	-29.18183811600375	0.86749204133106
H	35.90340640211188	-30.50451549322477	0.59531420149798
H	37.37662405873431	-29.91093293291578	1.37204867653067
H	36.43308882257700	-31.19128415424623	2.13584956987276
H	34.17610275122365	-22.50840631041426	10.59499372177699
H	32.67461289681534	-22.98640441047150	9.79263405744213
H	33.76510142652512	-21.84065969604198	9.01036973480267
H	37.38688708866485	-24.00243164454567	10.41543443937341
H	36.48515533086738	-25.29272065967007	11.21175643261548
H	40.22209326002352	-28.99141093106349	8.52525922441414
H	39.88447931342645	-27.29035565312073	8.87027214185257
H	38.90614565211457	-28.55354961971893	9.62046830903252
H	39.01255082924374	-30.95284664901824	5.75340531890110
H	39.97935164693764	-29.69426332880226	4.97760036014019
H	40.28184491739319	-30.12573726906604	6.66522179600057
H	35.90346675752738	-23.62601850033942	11.30168164339714
H	31.33189366528210	-31.82785998881544	5.96432125914348
H	32.40586428842743	-33.19758633365726	5.61924255534428
H	32.76074762575149	-32.11286246771633	6.97681641507785
H	34.26243401118733	-31.56335607961941	5.07321396794623
H	32.85970544256448	-31.32334153646086	4.00638742293150
H	32.50349240614673	-26.63365948877401	7.63331689938072
H	31.75695030398702	-28.14791212766652	7.08917999651633
H	32.86756444031843	-28.15708254332061	8.45744988762103
H	32.28172084518030	-26.91206950258448	2.07884900824980
H	37.56355126798790	-26.39938654469701	9.30505646005655
H	37.66291686713303	-29.78154600364208	3.91715741717399
H	32.39091921370558	-23.26417791472772	7.30202221792297
S	36.35802842472300	-25.06714041377638	4.49091226635106
C	35.87178023424416	-23.35148424455556	4.92121006878840
H	34.83260376862781	-23.14290962401184	4.64175209596687
H	35.98220287339291	-23.15497006828723	5.99394536631015
H	36.51937147498226	-22.65334557494342	4.37716826180120

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B3LYP Scan/Thiolate IPC Model/BSS/270 degrees Constrained Optimization

C	30.49237488742698	-24.87121175785362	2.62592840308132
C	36.35641161728843	-24.40410345065465	10.64566895127118
C	39.41460744702766	-30.03428201542325	5.90350304267472

C	33.51917393329217	-28.77650489261927	0.64345537240330
N	33.26657299021833	-25.60919652473118	5.04660484063411
N	34.93546558648347	-25.48376027534836	7.34226464732348
N	34.92679669201928	-27.71186691410393	3.95625268815622
C	32.90321877148691	-26.78826600440360	2.93017902810973
C	33.00246394461237	-24.04585489880852	6.91035108252327
C	36.89830994830666	-26.48092328032475	8.41615006970170
C	36.94205324377753	-29.04444202297972	4.32427291263245
C	30.57259327912800	-23.00468472451313	5.29025255816439
C	33.74027794569913	-22.75718811343142	9.63326317694998
C	39.35939019082723	-28.33130838179763	8.67825204635869
C	36.26962849110104	-30.25924025295377	1.54734152506612
C	32.57764207263402	-25.83301994831715	3.88831361850709
C	34.08136994917602	-24.47057884589464	7.68085775794683
C	37.25192391067304	-27.39708134347518	7.43255915952646
C	35.83562007606411	-28.65440818859384	3.57429996877272
C	31.45428691554221	-24.91297229121031	3.77683597569442
C	34.45299448790356	-23.89700761473757	8.96609723363357
C	38.41385825052333	-28.27357624716703	7.51514373926667
C	35.48016140424591	-29.21146515306235	2.27618255286627
C	31.48690538903137	-24.12728748130967	4.89736998274325
C	35.55203011246360	-24.59278965392518	9.39326177598279
C	38.43719100315202	-28.98926351727960	6.35132389721664
C	34.32585662717830	-28.58384362037230	1.89359176287597
C	32.62679461920208	-24.58092991276748	5.68085577601115
C	35.83815648725092	-25.58076880914153	8.36232401303032
C	37.28546654184221	-28.54714001213782	5.57679746807033
C	33.99897444089395	-27.64389034415653	2.95773023982074
N	36.59124453267931	-27.58791717905608	6.25381362374079
Fe	34.90047864700676	-26.63845704573832	5.67504667200010
C	33.57223611955497	-31.36975559974508	5.16859575128795
C	32.63413335552530	-32.22400592922544	6.01129356128364
C	32.59600513404772	-27.66226117446005	7.38763543772500
C	33.79900487416750	-27.94110261679370	6.52753964354212
C	34.04688423718623	-29.39529820107552	6.42937980534146
O	34.7428527774305	-30.05721104372632	7.17213310030375
O	33.35473330558578	-29.96809441406221	5.38990653400913
H	29.76520415320895	-22.86933293864603	4.56209832836042
H	31.10942351076158	-22.04841179215430	5.36435253774733
H	30.10368455456127	-23.18201515675289	6.26819641960371
H	30.99781547048611	-24.62881657717995	1.68064926352641
H	29.98989896176997	-25.83734267510665	2.47820209582745
H	29.71214084385273	-24.11771673654527	2.78034635126330
H	33.41029977218077	-27.83944038675681	0.08010433371502
H	33.98632778226762	-29.50687022277932	-0.02629441066606
H	32.50357434139757	-29.13478224106117	0.86356433675688
H	35.81041356651464	-30.51034146581679	0.58466391607583
H	37.29657997526170	-29.92558954454992	1.34365392874085
H	36.34734390386177	-31.19047252329560	2.12573395326357
H	34.18535879583338	-22.52006178935713	10.6060026681840
H	32.67842387993127	-22.98288354654954	9.80491693207646
H	33.77615254513974	-21.84225353467859	9.02523604046450
H	37.37879338242324	-24.06502196700841	10.42664479120882
H	36.44775360650749	-25.33826490611672	11.21663155624991
H	40.16034286974096	-29.05938182764952	8.50943859050834
H	39.83476014201433	-27.35870159489173	8.86734507407460
H	38.84530842639689	-28.62066464601098	9.60556084801570
H	38.92303783982786	-31.00252779331334	5.73418379326392
H	39.90567659359066	-29.75486224021245	4.96103133851086
H	40.20268738641740	-30.19399748261297	6.64770228727962
H	35.89980252450834	-23.66015054242384	11.30786535354818
H	31.59091441287834	-31.94859236421683	5.83021231367193
H	32.75521214278078	-33.28602149875969	5.76755291466498
H	32.84975692807358	-32.08871410090268	7.07273891243389
H	34.61495163642498	-31.60767289891452	5.38740494749164
H	33.39110257418262	-31.51255608176382	4.10087479530276
H	32.41918738715069	-26.59902261628844	7.53355344967946
H	31.68883920529075	-28.09981697079468	6.94043493817988

H	32.70883241423509	-28.12989204745043	8.37875061397000
H	32.25471510196575	-26.85055074921660	2.06115043449634
H	37.52863217630237	-26.44287244043726	9.29971786801175
H	37.58736881659703	-29.80677194715947	3.89816251521584
H	32.40462421964207	-23.22765033741400	7.30072931961883
S	36.36698484169306	-25.06515827744682	4.51087126384099
C	35.85625616362569	-23.34401769696963	4.88822219719137
H	34.82531736674393	-23.14820106936749	4.57126450084465
H	35.93138375537437	-23.12312311287369	5.95931522638841
H	36.51645678861365	-22.65377896117671	4.34930346651362

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B3LYP Scan/Thiolate IPC Model/BSS/280 degrees Constrained Optimization

C	30.48659930943880	-24.81792902481175	2.61480062453288
C	36.33821215735922	-24.44269562152762	10.64798883825324
C	39.35176749661144	-30.08261312956193	5.88754521426826
C	33.48181836155604	-28.74070948127518	0.61955549654501
N	33.25504495243734	-25.58625029810864	5.03256691979524
N	34.92095434254271	-25.48483685394985	7.33132041635364
N	34.89445318187769	-27.70179115791795	3.93842768656421
C	32.87931699080995	-26.75805945193607	2.91442499674674
C	33.00649447411411	-24.02310327031128	6.89889762259992
C	36.86628189390321	-26.51279983661994	8.40869681628746
C	36.89487764025377	-29.05692263907356	4.30415404509360
C	30.58807219311946	-22.95426587689184	5.28081452274748
C	33.74659886197674	-22.75906217629245	9.63286423564254
C	39.30535770328481	-28.39327086614192	8.67050185079267
C	36.22387977502073	-30.24299480960872	1.51528759860363
C	32.56311024984651	-25.80161277950501	3.87456830112740
C	34.07754069265620	-24.46391937720706	7.67162147136760
C	37.21200168807473	-27.42996126563992	7.42316326362545
C	35.79645977358472	-28.64900671039815	3.55256145738759
C	31.44941542374471	-24.86969585613700	3.76445490916893
C	34.44991113270579	-23.90242128049059	8.96199022950922
C	38.36365234522467	-28.31981135689325	7.50525930387272
C	35.43937186201885	-29.19579001204222	2.25048420441471
C	31.49136445089491	-24.08481391575017	4.88525728081842
C	35.53855871499339	-24.61360168450691	9.39011870175375
C	38.38296709010025	-29.03043329341151	6.33797449977022
C	34.28948403875012	-28.55914106545252	1.87057309167140
C	32.62660181759009	-24.55132957946615	5.66782723143652
C	35.81779996272887	-25.59910253548745	8.35484362920260
C	37.23854608909053	-28.57215897650786	5.56202678446824
C	33.96817545360955	-27.62256211125505	2.93952303705569
N	36.55257611220343	-27.60860619370632	6.24168642197837
Fe	34.87461031269830	-26.63437147718850	5.66063347276035
C	33.84786300117499	-31.41137447288173	5.30334272683637
C	32.82413995052187	-32.26592413374183	6.03906401089185
C	32.55357169821067	-27.62417820352350	7.37257879000777
C	33.76082920027989	-27.92174430517935	6.52431592867856
C	34.05072577176556	-29.37118853377147	6.52861545244713
O	34.62977618844895	-29.97422754919346	7.41082982958864
O	33.55690905037854	-30.01040485917902	5.42216595727626
H	29.78689715045109	-22.80401733953919	4.54879456034749
H	31.13579218499183	-22.00513913525264	5.36538790133028
H	30.11093599094360	-23.13326078725787	6.25450845976545
H	30.99394365446656	-24.58492679577339	1.66819217705627
H	29.97078025994732	-25.77753467581239	2.47030424514454
H	29.71675270980682	-24.05367015173174	2.76837164935073
H	33.36984682525734	-27.79810644671303	0.06627377631346
H	33.94971476456305	-29.46288441858392	-0.05852206873560
H	32.46735801938185	-29.10395233603039	0.83714555749244
H	35.76633136181355	-30.48228644389776	0.54881796160244
H	37.25384439664957	-29.91475932501444	1.31807815163207
H	36.29347851372891	-31.18024505929231	2.08506657713851
H	34.17586280354039	-22.54626148721755	10.61826416158957
H	32.67731117174239	-22.96640752046723	9.77896156418488
H	33.81300625513409	-21.83523523707493	9.04084600259004

H	37.36050686765086	-24.09724773508342	10.43828369872256
H	36.42960604103168	-25.38584656058114	11.20363101095878
H	40.10074506731545	-29.12682887747158	8.49907025733914
H	39.78814767765451	-27.42591903985942	8.86732250401264
H	38.78599881038807	-28.68468365252166	9.59416661155112
H	38.85511117781807	-31.04957682498666	5.72485390850055
H	39.83758725306516	-29.80905785257583	4.94075166968437
H	40.14413329344031	-30.24333391674715	6.62689369458356
H	35.87741144081430	-23.71072527242038	11.32060699020820
H	31.81097169657090	-32.03859735428075	5.69446421195681
H	33.01403320682911	-33.33130144792816	5.86377122978735
H	32.87677802771501	-32.07983137536306	7.11318531389009
H	34.85438597303264	-31.60012920061635	5.68127628539833
H	33.82745653846357	-31.60555758369840	4.22863507635819
H	32.35164790791162	-26.55938679965827	7.46191706464873
H	31.65449605429344	-28.10549277075540	6.95335052058196
H	32.68161096448655	-28.03810533427383	8.38473420408543
H	32.23048053453341	-26.81213272781206	2.04506967322136
H	37.49357885535132	-26.48657932030232	9.29480493528574
H	37.53446845740010	-29.82232891274594	3.87478558155076
H	32.41711334790126	-23.19945840485549	7.29056990022662
S	36.36992542706837	-25.07517885390876	4.51581650175937
C	35.85515230526993	-23.34922105386741	4.86532483652173
H	34.83056879834078	-23.15494473497295	4.52761398983181
H	35.91179736756580	-23.11656034287927	5.93504021829936
H	36.52622444006614	-22.66587786763105	4.33095956229069

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B3LYP Scan/Thiolate IPC Model/BSS/290 degrees Constrained Optimization

C	30.50430023319574	-24.64568210621990	2.58623126894985
C	36.28315867282286	-24.59252128392840	10.67968950027744
C	39.25125659114483	-30.14205753866507	5.79339526731904
C	33.36714025017712	-28.66309870281081	0.57761354421530
N	33.24124857979102	-25.52411355526602	5.00252919117095
N	34.88253594809757	-25.51544489676253	7.32259354368824
N	34.81144499674406	-27.68002339746782	3.90000892017350
C	32.82307771593891	-26.67526808634654	2.88161906748450
C	33.03074239115794	-23.97665862339839	6.88675988980140
C	36.77940998461234	-26.62630044926060	8.40445321711547
C	36.79717927144632	-29.06557603983537	4.23526530291807
C	30.67077008474940	-22.79731273466244	5.26014755267587
C	33.76855354537561	-22.79470025525837	9.65707025580761
C	39.19392368062582	-28.54306576263598	8.63085823809484
C	36.08789188872363	-30.21817061618160	1.44567878659196
C	32.54307908187542	-25.70846001971592	3.84340298308770
C	34.07076398842984	-24.47242206842356	7.66893666170984
C	37.11495597632739	-27.52949795341620	7.40207340984688
C	35.69912651850856	-28.63493604940241	3.49822071974176
C	31.46423396125166	-24.73595918980305	3.73579184113484
C	34.44361649663930	-23.94826210164842	8.97489719222531
C	38.25703125166187	-28.43164659711146	7.46469054786747
C	35.32821954159881	-29.16061305157298	2.19151673384687
C	31.53356444678149	-23.95780517225312	4.86011267293397
C	35.49862599814129	-24.70663154741766	9.40597307330277
C	38.27789890456800	-29.10776888821014	6.27581241776948
C	34.18659302051721	-28.50361607571819	1.82379027967203
C	32.64791795473160	-24.47093820769672	5.64309614221664
C	35.75916035567404	-25.68177078563584	8.35655885563879
C	37.14013336186994	-28.62018497362428	5.50849538385650
C	33.88553954908629	-27.57191829627402	2.90313508323122
N	36.45633883514125	-27.67314430497117	6.21454362408638
Fe	34.81368872557489	-26.63615494990984	5.63689249454092
C	34.49492916230556	-31.43371528027982	5.84611585705663
C	33.36505720122075	-32.38691486145207	6.21060815840620
C	32.31004092633080	-27.58449189356194	7.11666363586893
C	33.64773520025293	-27.89000054734431	6.49750141564086
C	34.04597482687725	-29.28388989444818	6.78174130690877
O	34.37226677462539	-29.70574626337860	7.87584807421508

O	34.01303900368933	-30.09229157545438	5.67919692898641
H	29.87614026304612	-22.61586633970024	4.52820628994592
H	31.25173404415918	-21.86860092958555	5.34892468126078
H	30.18683631242153	-22.96342621616325	6.23268853274884
H	31.01659218881562	-24.40918838491058	1.64306766754695
H	29.96861582729090	-25.59199023813752	2.42742702180895
H	29.75029320802732	-23.86815981327262	2.75143534726659
H	33.27598633090393	-27.71797519241287	0.02464992475172
H	33.81122802585700	-29.39751631278761	-0.10329268046888
H	32.34491625718353	-28.99968471074953	0.80184209556764
H	35.62395344181343	-30.43854808646395	0.47779403670424
H	37.12511640113473	-29.91251856942020	1.25034528609596
H	36.13548246516181	-31.16211860888876	2.00694514551036
H	34.22249554661217	-22.58290943383253	10.63149457023963
H	32.70036077994773	-22.98923005656713	9.82832870792411
H	33.83183351511774	-21.87445709195719	9.05947826376874
H	37.33810094572152	-24.35248495370764	10.48667346592672
H	36.27088808783507	-25.53056014066594	11.25155917056065
H	39.98608841166170	-29.27599188912349	8.44252738076480
H	39.68137449905437	-27.58411120981829	8.85487390111958
H	38.66886798881546	-28.85564724280681	9.54423664207584
H	38.75471009676124	-31.09519131769122	5.56332847576757
H	39.76319492250233	-29.81957956867868	4.87609702954331
H	40.02286244371260	-30.34899396210776	6.54302782946227
H	35.88205260295274	-23.80750207225641	11.33034753564786
H	32.55606789729708	-32.32502012981627	5.47697194426210
H	33.72682496412313	-33.42145237887726	6.23673006439371
H	32.96136032988887	-32.13918155747309	7.19465592382324
H	35.27266953048260	-31.44184441725157	6.61124716215708
H	34.93793884161968	-31.69334154336311	4.88191389452248
H	32.06650457223213	-26.52496042262996	7.10009811902124
H	31.50755449951408	-28.11880395072648	6.58120712953052
H	32.27563464606368	-27.93635760381424	8.15815627955970
H	32.17246494730112	-26.70587122329998	2.01244519103289
H	37.39691914193112	-26.63394906553630	9.29766321812690
H	37.43307175354294	-29.82199768951934	3.78486691517156
H	32.46744139663528	-23.13782366329984	7.28447682618518
S	36.39728108657929	-25.11153299679280	4.56322843639936
C	35.82570567510728	-23.37924318663955	4.75787655664763
H	34.83094736511674	-23.22657292721731	4.32406478439468
H	35.78740123478205	-23.08233624027709	5.81249509808333
H	36.52980761298917	-22.71596106433599	4.24108409507188

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B3LYP Scan/Thiolate IPC Model/BSS/300 degrees Constrained Optimization

C	30.46305569683247	-24.69375861466363	2.61643002987740
C	36.28306290249850	-24.59150936632683	10.67688562061181
C	39.26168297412091	-30.12677437211912	5.78661317274151
C	33.34910037478933	-28.68865494431627	0.59265749376156
N	33.22945786387925	-25.53842198027868	5.01062395769115
N	34.88147704751367	-25.51732708982307	7.32074215690441
N	34.79815420008697	-27.69536751743254	3.90988267112735
C	32.79198764271506	-26.71253677753713	2.90614261490040
C	33.04658013923925	-23.96135735053729	6.87268130835266
C	36.76303817435198	-26.64298874407763	8.41446321342937
C	36.80324981258320	-29.05598983592671	4.23035549494956
C	30.66809901084648	-22.80321103294483	5.25873043067164
C	33.80588034615753	-22.75764663699040	9.62825187783621
C	39.18200244255137	-28.55478592285098	8.63847351886804
C	36.10311184973441	-30.19778523380347	1.43432262721574
C	32.51767659216009	-25.73877415141491	3.86231340241608
C	34.08544630144782	-24.45817133754943	7.65604471547884
C	37.09846026394487	-27.54713150946650	7.41239474560282
C	35.69856724368743	-28.63378500577621	3.49843833259987
C	31.43860744719974	-24.76646630286602	3.75394939555361
C	34.46476050456160	-23.92708339793478	8.95721173467751
C	38.24585534787942	-28.44275430221863	7.47165274079282
C	35.32925639110760	-29.15837915945584	2.19102504296335

C	31.52459879319419	-23.97016190363115	4.86421874768231
C	35.50515111418544	-24.69955417692993	9.39865714964791
C	38.27611864424178	-29.10745948486674	6.27630701536701
C	34.17332539668864	-28.52037474396509	1.83446421936576
C	32.64749215942273	-24.47352543497868	5.64134598130246
C	35.75317630280123	-25.68769383803651	8.35842109049857
C	37.13686854018703	-28.62251714607215	5.50984520345972
C	33.86467050828487	-27.59772402680977	2.91963990350636
N	36.44285034180415	-27.6876202027579	6.22260732290196
Fe	34.80236264931099	-26.64848465049885	5.64289207255367
C	34.53640417592245	-31.40994117221067	5.82382439835194
C	33.38720836493881	-32.37576974172718	6.07769044274796
C	32.33177672423477	-27.52462002605654	7.20345831078705
C	33.62352345404700	-27.89073917237312	6.52164262816155
C	33.97111964055239	-29.30085425326493	6.78259800750884
O	34.16092591067321	-29.77403003990171	7.89050579620980
O	34.06891997382325	-30.06442361692253	5.65448220424917
H	29.87804793662553	-22.61706869762734	4.52306735981333
H	31.25530454877683	-21.87872042525115	5.34899054558559
H	30.17855733357348	-22.96469879035874	6.22935088310692
H	30.96525351347344	-24.49379105923573	1.65960225523155
H	29.90943581792152	-25.63516292486074	2.49338764941621
H	29.72442560566611	-23.89924242717273	2.76953776935234
H	33.22702918421535	-27.74000797140333	0.05202859833202
H	33.80907611357437	-29.40182352562019	-0.10017723689267
H	32.33864682499101	-29.05743584888708	0.81980381676637
H	35.64502461163736	-30.41061111628854	0.46197504802283
H	37.13729122160021	-29.87754995691573	1.24669074003007
H	36.15971842568843	-31.14873622538116	1.98288912340380
H	34.28916554809283	-22.51786296347048	10.58188117666531
H	32.74431362788185	-22.95081389234072	9.83860585561617
H	33.84668942344960	-21.85459073644315	9.00355154877169
H	37.35466118488841	-24.44039447076207	10.48757543285257
H	36.19408421907477	-25.50095284995348	11.28754220539826
H	39.97330840330032	-29.28881630381984	8.45094038023556
H	39.67068665311273	-27.59631755296607	8.86216812503035
H	38.65644388821301	-28.86605569730654	9.55198964864197
H	38.77531175671308	-31.08085234776074	5.53964524631856
H	39.77699491307744	-29.78661355381643	4.87761354027703
H	40.02998950214018	-30.33733082853308	6.53863672973924
H	35.93622884864121	-23.75165113142218	11.28922165954142
H	32.63308627118874	-32.29378923278460	5.28936279265660
H	33.75137274038791	-33.40973762847594	6.09766183846643
H	32.91354057794578	-32.15879096398857	7.03719712520217
H	35.25660093587078	-31.43817193560612	6.64324725392183
H	35.05004561096101	-31.64328060373152	4.88849825489914
H	32.19043071137096	-26.45081514583396	7.30017832621713
H	31.47475519332945	-27.91490957405693	6.62925111581433
H	32.27500600466935	-27.98083355415139	8.20091609982143
H	32.13300359155242	-26.75281035635023	2.04366753207440
H	37.37784782941078	-26.65274650097962	9.30948193755710
H	37.44942641341893	-29.79926469387339	3.77269100284173
H	32.49316931741266	-23.11235213430892	7.26251975083153
S	36.37805752217889	-25.13621754322213	4.53686119254278
C	35.85725937650390	-23.39478547918596	4.78379758248900
H	34.85248152831794	-23.21009166068968	4.38665414647683
H	35.86116537736298	-23.11649232098361	5.84414518350479
H	36.55948362758649	-22.73893213934796	4.25518097010055

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B3LYP Scan/Thiolate IPC Model/BSS/310 degrees Constrained Optimization

C	30.44784420938013	-24.70315100001131	2.62437240074511
C	36.28825611728455	-24.58802649921162	10.66865749460984
C	39.25145279091892	-30.13139706822599	5.78145009327302
C	33.32576579045794	-28.70295982813921	0.60156462592006
N	33.21567662705532	-25.54842132074257	5.01663598614161
N	34.87707088499516	-25.52058543791563	7.31839154923531
N	34.78023577151487	-27.70763845379566	3.91570454261534

C	32.76703306359885	-26.73201775484693	2.91955718058283
C	33.05087090789679	-23.95500480508981	6.86583170414661
C	36.74930011360473	-26.65646783664570	8.41761455712373
C	36.79951423912625	-29.04987880087757	4.22248655529246
C	30.67414949318433	-22.79378407003331	5.25128345428292
C	33.82647881617982	-22.73836562645905	9.61032515923429
C	39.15994957657065	-28.57959662274584	8.64415585187083
C	36.09697502897941	-30.18990747052422	1.42658972463076
C	32.49874692102476	-25.75316533264801	3.87220268589810
C	34.08949426799973	-24.45317847773241	7.64872946212316
C	37.08278387137234	-27.56171930011008	7.41568031466705
C	35.68844981996976	-28.63498167481430	3.49642101155157
C	31.42492142766327	-24.77538197986649	3.76062081670560
C	34.47474448655932	-23.91766902785796	8.94623176277429
C	38.22949717110181	-28.45831895790547	7.47367919446446
C	35.31799597894452	-29.15871302007823	2.18909245523456
C	31.52005902521172	-23.97096481526378	4.86430844876704
C	35.50816837991680	-24.69721561788420	9.39184865368765
C	38.26507758833990	-29.11388295193890	6.27320831982583
C	34.15380434573525	-28.53142930399030	1.84040345868717
C	32.64228202549932	-24.47540621090219	5.64132483968654
C	35.74738294540797	-25.69299545369012	8.35697904427381
C	37.12802414255880	-28.62501410198913	5.50613984830037
C	33.84243619791073	-27.61415707940120	2.92949441843836
N	36.42962441403043	-27.69745721555506	6.22381284433842
Fe	34.78980179152862	-26.65805216466296	5.64628495538539
C	34.63669703931183	-31.39254926596682	5.90064487530773
C	33.46626093510910	-32.36457296486530	5.96851101458682
C	32.33033891232475	-27.48512964171385	7.24248877505221
C	33.59958820572633	-27.89808050948903	6.54369623655047
C	33.91624803770442	-29.31146790692840	6.81534374918469
O	33.94460731958824	-29.81666301284220	7.92774650892220
O	34.19278489898841	-30.04573388812418	5.69834647659069
H	29.88455353692512	-22.60653714784173	4.51542941260904
H	31.26939157658780	-21.87370591769696	5.33336417261549
H	30.18484127452153	-22.94362203287395	6.22385635029366
H	30.95044805333341	-24.51632728338289	1.66512869173939
H	29.88481977321657	-25.64008966203407	2.51029905811121
H	29.71736166995336	-23.90011336352299	2.77183709613851
H	33.20143935489619	-27.75563342310324	0.05901964629465
H	33.78410081783461	-29.41746488674594	-0.09095954823194
H	32.31627878733941	-29.07181035562037	0.83260788057416
H	35.63911829079498	-30.40082480437103	0.45370798556876
H	37.12911385523685	-29.86308520645434	1.23939311801324
H	36.15899576609847	-31.14284322891299	1.97107803922160
H	34.30687168194859	-22.50203858747987	10.56623374595937
H	32.76141885581404	-22.91800018067370	9.81452201216815
H	33.88228559983079	-21.83748720474192	8.98354985829474
H	37.35923657399927	-24.43458177625114	10.47741519333509
H	36.20217874969669	-25.49784048520793	11.27903435137211
H	39.95313376865152	-29.31089318763051	8.45403278425414
H	39.64626081632047	-27.62259146970249	8.87898045642660
H	38.63031970844513	-28.89960226755192	9.55234272330264
H	38.76575440654180	-31.08557630643004	5.53343169265038
H	39.76587454250953	-29.78949496541616	4.87266155432738
H	40.02042689658747	-30.34226435480427	6.53270194106437
H	35.94079797381886	-23.74910856084114	11.28189113046595
H	32.83212866744347	-32.26719796051545	5.08252208905708
H	33.82672453014315	-33.39867150600971	6.02149998744175
H	32.86025069286896	-32.16494758808310	6.85443605132008
H	35.23411913284584	-31.44235968921382	6.81284618733120
H	35.27707333279599	-31.60365560123758	5.04132845566718
H	32.29547591657170	-26.41987498185993	7.46158236416701
H	31.46045337813938	-27.70637024311953	6.60227990965648
H	32.19257746784821	-28.04467771884786	8.17545284046920
H	32.10460468067435	-26.77488447593068	2.05985499471912
H	37.36267424283607	-26.66850038213435	9.31359919647294
H	37.45217616710833	-29.78385788302148	3.75897310324451

H	32.50457172028661	-23.0995453266259	7.2514777925333
S	36.36260959935008	-25.15397568231193	4.52718380705180
C	35.85864297612633	-23.40911631730414	4.78220382367040
H	34.85250224988344	-23.21508264852724	4.39301337003334
H	35.87281580773596	-23.13363844974765	5.84317757249378
H	36.56266852616366	-22.75828140869615	4.24986505739323

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B3LYP Scan/Thiolate IPC Model/BSS/320 degrees Constrained Optimization

C	30.44129612540087	-24.68883887467099	2.63184877947293
C	36.27537671725729	-24.63550697159424	10.67815191426583
C	39.26121312182343	-30.11626960121501	5.73842817037584
C	33.29274231142049	-28.70824450700881	0.60077849502695
N	33.22231368503031	-25.53968562261669	5.00664862915854
N	34.87536766282277	-25.53660580191420	7.31442333633518
N	34.76454335169734	-27.71355264278278	3.90715781104576
C	32.75334489208894	-26.72854983969395	2.91675983956703
C	33.06218635252920	-23.95502864338950	6.86369772249206
C	36.73801547762512	-26.68800282803070	8.41338864936500
C	36.79093987092549	-29.04809499483139	4.19945416489695
C	30.68606767331572	-22.78208350304521	5.25916489558511
C	33.83398549633741	-22.76023702678446	9.61823387603511
C	39.15979439433941	-28.59852491722792	8.61850224394117
C	36.06874406496563	-30.19486586106958	1.41111290431229
C	32.49756512058694	-25.74369849005683	3.86711484650661
C	34.09428438429986	-24.46462629296595	7.64740434917627
C	37.07289038055438	-27.58383513943271	7.40347490584116
C	35.67178552352816	-28.63972243618250	3.48259030501635
C	31.42530842559365	-24.76345206830771	3.76200946189511
C	34.47712715776827	-23.93988598394578	8.94978411984575
C	38.22542108269376	-28.47382837217796	7.45138963144536
C	35.29408148782605	-29.16334446862562	2.17744360595613
C	31.52827327591958	-23.95995464130516	4.86602585724986
C	35.50220726045899	-24.73017297827964	9.39597249642578
C	38.26477068810018	-29.11491534619893	6.24322878600372
C	34.12768059534820	-28.53641086040958	1.83493690963766
C	32.65292567057721	-24.46765573559308	5.63677435414440
C	35.73976120915223	-25.72070119462160	8.35611026536202
C	37.12217299104793	-28.62697265717810	5.48351783211311
C	33.82279724104380	-27.61794704418481	2.92468170406941
N	36.41856367413698	-27.71176817319622	6.21147163407381
Fe	34.78375664926901	-26.66374089936606	5.63634939823925
C	34.75792447234831	-31.37107806593663	6.11508553613678
C	33.59893161080641	-32.35145939881931	5.98524931007289
C	32.26717792433116	-27.42807160966220	7.15166685849093
C	33.55543610728026	-27.89666866447099	6.52425801868637
C	33.83922041812942	-29.30061618276596	6.85392976558573
O	33.64955106868936	-29.81223857181618	7.95019124466324
O	34.35355816382330	-30.02998614573166	5.82115176927807
H	29.89095112466453	-22.59466489406602	4.52939944039283
H	31.28243156924277	-21.86231178486466	5.33637625751037
H	30.20438200792433	-22.93161115924509	6.23550077258283
H	30.93733578195419	-24.49456563478861	1.67063912888241
H	29.88149745139778	-25.62737893719068	2.51603443481280
H	29.70844018780614	-23.88970481868036	2.78833728222732
H	33.16627436118596	-27.76125755934832	0.05815475408088
H	33.74653804924622	-29.42379978548623	-0.09361300837771
H	32.28422008943057	-29.07593643072168	0.83776427952946
H	35.60603910085009	-30.40557645344110	0.44049085257897
H	37.10002080560520	-29.86829732064443	1.21881251654606
H	36.13285089842469	-31.14747866538060	1.95570696226997
H	34.31320148258368	-22.53165963357714	10.57658901093971
H	32.76741394682174	-22.93477831504170	9.81879121979867
H	33.89671175086411	-21.85653987984591	8.99624669452134
H	37.34957160259862	-24.49642483161934	10.49433741708257
H	36.17244912839376	-25.54572101518642	11.28530751198849
H	39.95491356282155	-29.32601525784466	8.42203853375240
H	39.64350959973365	-27.64113171450228	8.85707923507426

H 38.63439521913534	-28.92510242027005	9.52684695797883
H 38.78703296581084	-31.07441188166088	5.48332043228717
H 39.76778270793386	-29.75934564847218	4.83108648061027
H 40.03559378283462	-30.32434492790536	6.48488390677241
H 35.93568302135639	-23.79355857975145	11.29156519452497
H 33.13800721113684	-32.27354063636437	4.99629448612231
H 33.94793081580667	-33.38177754765267	6.12248476021621
H 32.83990872345618	-32.14157182994651	6.74101520942517
H 35.18521200659988	-31.40951660628988	7.11905585239252
H 35.54126819907484	-31.58716562011507	5.38476070577494
H 32.39426894040022	-26.48762301150889	7.69371548482812
H 31.52289202083309	-27.22335895428785	6.36979430010497
H 31.84856996043911	-28.16760863633267	7.84159431741470
H 32.08572578078425	-26.77046612467013	2.06105131438082
H 37.34966555774111	-26.70780850877066	9.31037926680355
H 37.44631769576956	-29.77533087429025	3.72915902026094
H 32.51951464144915	-23.09888903509299	7.25286019233091
S 36.37236902574242	-25.16847293471179	4.53060395476944
C 35.85800196867249	-23.42381515644502	4.76265748126608
H 34.85505937645560	-23.23840530540918	4.36133540439716
H 35.85967363727939	-23.13846458461029	5.82114377993447
H 36.56475545884565	-22.77500102685974	4.23155080341879

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B3LYP Scan/Thiolate IPC Model/BSS/330 degrees Constrained Optimization

C 30.43870201198257	-24.68645849098529	2.63545329284628
C 36.26321271471664	-24.65695617453580	10.68670492863912
C 39.27496623311995	-30.09546665244426	5.71629341299947
C 33.26897011764839	-28.72428518888936	0.61176736900495
N 33.21989605633294	-25.54410153236238	5.00767041939946
N 34.87475114860864	-25.54306619154095	7.31435022533304
N 34.74794838075508	-27.72877600163406	3.91466719634830
C 32.73581246656985	-26.74256712889940	2.92695825289269
C 33.07367260272698	-23.94940521157132	6.85756231617264
C 36.73011329515073	-26.70296480725915	8.41623125874284
C 36.78771724706863	-29.04549509794848	4.19294295021230
C 30.70591853101861	-22.76527195325931	5.25007264317133
C 33.84209600682966	-22.76181248852415	9.61598307245965
C 39.16291021237507	-28.60188272531935	8.60846261122175
C 36.05568412678412	-30.19847479504237	1.40878960625987
C 32.48986613749138	-25.75004990306784	3.87184365397927
C 34.10016751226387	-24.46536227921717	7.64438822367543
C 37.06899723110320	-27.59162927776034	7.40100620409026
C 35.65880625958874	-28.64936272561595	3.48484082902951
C 31.42493943304660	-24.76218886632223	3.76359912351993
C 34.48082999197810	-23.94453543768357	8.94878756544356
C 38.22710708525861	-28.47512457415043	7.44273525140522
C 35.27766458412589	-29.17397376733477	2.18120240725342
C 31.53764138391408	-23.95230032326966	4.86203261930910
C 35.49754749942738	-24.74314867278762	9.39947877035200
C 38.27079443455511	-29.10607213629862	6.22949862943741
C 34.10656889938030	-28.55232107189254	1.84418261707462
C 32.66009871781459	-24.46416899113954	5.63303850126623
C 35.73399697217070	-25.73342218676817	8.35925970122730
C 37.12330194615063	-28.62165724624539	5.47475540651762
C 33.80283550925215	-27.63507702355465	2.93502161370823
N 36.41563980931166	-27.71498991376128	6.20867568730413
Fe 34.77738573322664	-26.67249961011654	5.63876988214837
C 34.80272278354514	-31.36486604455997	6.23971847735652
C 33.66795477488954	-32.3208452056439	5.89142743606428
C 32.25765856437776	-27.40088684190038	7.16243007219509
C 33.53741598474038	-27.90173969646215	6.54339440092574
C 33.78055654882247	-29.31111337674442	6.88305917134434
O 33.41498074409988	-29.86160894054779	7.91657564290521
O 34.46755459427873	-30.00960694716242	5.93218956078479
H 29.91510086916380	-22.57142131618006	4.51735092102379
H 31.31120020919992	-21.85140612776943	5.32733552491587
H 30.21955461163940	-22.90802975064063	6.22511682739793

H	30.93403318629204	-24.50282106541609	1.67179611734750
H	29.87044135205960	-25.62078463571202	2.52726903260694
H	29.71328566232431	-23.87993359325457	2.78857486265478
H	33.14672644462203	-27.77853324929766	0.06591682709153
H	33.71811699567785	-29.44454490766863	-0.08075935684943
H	32.25887396797491	-29.08573276708081	0.85135091151715
H	35.58575626071979	-30.41546913628799	0.44303158555105
H	37.08137139860121	-29.86089275776958	1.20581039997146
H	36.13550634548243	-31.14923985254726	1.95428258490156
H	34.32089696311919	-22.53522422020926	10.57500313270427
H	32.77446321261340	-22.93156742274985	9.81496219903095
H	33.90984306598079	-21.85860071671759	8.99386283224720
H	37.34040608680551	-24.53268239354635	10.51020881100512
H	36.14366889869650	-25.56485177981511	11.29436735217021
H	39.96095216557055	-29.32493931177666	8.40753960674208
H	39.64266195973691	-27.64372138050575	8.85189602324605
H	38.63978241530913	-28.93554506599583	9.51559333949907
H	38.80894459913043	-31.05563359155806	5.45375557572201
H	39.77781325080283	-29.72709077574567	4.81147217316988
H	40.05155775615173	-30.3029877668197	6.46058595461601
H	35.93074012962163	-23.80966901935298	11.29670002663238
H	33.36830775800500	-32.19467768582662	4.84704577496774
H	33.98147221431532	-33.36144547751681	6.03681586750124
H	32.80265496291030	-32.12932428483837	6.52831164722468
H	35.06317738342025	-31.44500905980303	7.29721355844861
H	35.68928332036620	-31.57154855508739	5.63536964961344
H	32.40867798433029	-26.47022718270052	7.71505590672533
H	31.52919658597852	-27.16323177238821	6.37539156827553
H	31.80973754467735	-28.13512969529981	7.83790992087721
H	32.06543632663680	-26.78553886808946	2.07347023982027
H	37.33962740862644	-26.72709641990229	9.31457633054023
H	37.44636513646093	-29.76679196057443	3.71810449775575
H	32.53704834431517	-23.08807544489552	7.24359484023387
S	36.36631910020117	-25.18412331310548	4.52554633243860
C	35.85612227653313	-23.43721335734122	4.74823792166436
H	34.85432183321780	-23.25082220931327	4.34452381611923
H	35.85692472559482	-23.14713344314553	5.80540409558904
H	36.56571000061295	-22.79303014074856	4.21530076326824

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B3LYP Scan/Thiolate IPC Model/BSS/340 degrees Constrained Optimization

C	30.38855244230442	-24.79547461548799	2.69800256342623
C	36.32096679980101	-24.55984288632490	10.66531881327227
C	39.30508716067158	-30.07473309730975	5.77183631287866
C	33.25654100837968	-28.81485533885583	0.69014220689044
N	33.21481731246634	-25.57570075095783	5.04272892822321
N	34.89612462843742	-25.52198115747564	7.32892280570322
N	34.75191261519001	-27.76315847601854	3.96792821500764
C	32.71268059466296	-26.82092468755998	2.99379835743793
C	33.08965760767787	-23.93859917666673	6.85649037571566
C	36.75685170157187	-26.66268771649871	8.44140894920166
C	36.81116417327675	-29.04899599408363	4.24362596966942
C	30.68754925435770	-22.80788777675338	5.25896910383386
C	33.89450554700708	-22.68309303420704	9.57494072382303
C	39.19383187215566	-28.55362513734802	8.64898006870101
C	36.08466699913413	-30.22246030880391	1.46535708569305
C	32.46880620516992	-25.81378839758887	3.92350670600062
C	34.12701066812152	-24.43415410364221	7.64140607093134
C	37.08916403810428	-27.56831283762559	7.43908416464640
C	35.67468980122356	-28.67035624539777	3.53699238398938
C	31.39424245805167	-24.83706535150743	3.81064131410549
C	34.52202354237790	-23.88390197726331	8.92947037054493
C	38.25233549482867	-28.44513041918717	7.48590849756691
C	35.29076721694160	-29.21257116096076	2.24139928535096
C	31.51999549382963	-23.99946326339546	4.88675581892528
C	35.54018059764139	-24.67556837201137	9.38945895591110
C	38.29584397595293	-29.08729457284327	6.27881330303278
C	34.10271707542435	-28.61794814272917	1.91297737470817

C	32.65875917952794	-24.48484689356024	5.65114520266163
C	35.76354645048717	-25.69088758045503	8.37048707867149
C	37.1428787232179	-28.61735073068793	5.52322869495847
C	33.79437674185173	-27.69606249490815	2.99869816419569
N	36.43134577017010	-27.70850414535746	6.25151308677421
Fe	34.78443282849468	-26.68417872568237	5.67739059107946
C	34.67726374239442	-31.39009907501597	6.10365976297901
C	33.59110721030626	-32.20361698591407	5.40981886762297
C	32.30330046603621	-27.36635538858565	7.27922967707741
C	33.53737405917441	-27.90422698253458	6.60252212318386
C	33.66816293288805	-29.35354234696808	6.82340701777124
O	33.12157395814663	-29.99151000337349	7.71934576459943
O	34.47775675958045	-29.98727192314206	5.92531381494452
H	29.87310775153918	-22.64717488494209	4.54435479814721
H	31.28501487231063	-21.88596430730508	5.28642496124777
H	30.23244573637316	-22.92195452654398	6.25256842399523
H	30.86479962960001	-24.61876271555157	1.72346103527719
H	29.83471593185236	-25.74076667427482	2.61395394133240
H	29.65205723273195	-23.99893758585377	2.85048763865276
H	33.12752109464131	-27.87977976237126	0.12756042223362
H	33.70289920109605	-29.54680780453100	0.00816633025594
H	32.24949718727945	-29.17461472764963	0.94405185068464
H	35.60379707393508	-30.46352862828480	0.51076386175162
H	37.09580399934884	-29.85635972907058	1.24004523436195
H	36.20323644429957	-31.16440242555234	2.01881676729676
H	34.38300081394574	-22.43714230689422	10.52428369296038
H	32.82798667399205	-22.84311421402774	9.78729622535314
H	33.96084439214503	-21.79468965090818	8.93178116691555
H	37.39498142233217	-24.43096230463339	10.47299479801467
H	36.21626927027169	-25.45691207118525	11.29155758598476
H	39.99149904332183	-29.27905485648181	8.45524875196804
H	39.67420981306228	-27.59163465977886	8.87583488255409
H	38.67565989523745	-28.87388270531748	9.56378077328364
H	38.84329067584326	-31.03758496940740	5.51202243800551
H	39.80876734906079	-29.70797478349627	4.86676295539100
H	40.08087263216859	-30.27631805927578	6.51865535253473
H	35.98974857472990	-23.70374625015397	11.26358618057961
H	33.51675355572198	-31.91950972776734	4.35644010370969
H	33.81666495062547	-33.27532363901359	5.46399733168779
H	32.62463338134018	-32.03036947185206	5.88687882523578
H	34.71077868642466	-31.62228856570513	7.17028718037078
H	35.65659594856189	-31.58784801413240	5.66068064306673
H	32.50456105874531	-26.44061086814002	7.82157806845298
H	31.54601938883035	-27.11070657095772	6.52491145393100
H	31.86266980418793	-28.09181678390059	7.96767649923516
H	32.03042991668769	-26.88746090441476	2.15130359507803
H	37.37300624049899	-26.66993145219951	9.33556997921589
H	37.47739593658062	-29.76453991556821	3.77063965967723
H	32.55675640524072	-23.06893638493344	7.22871712090142
S	36.33621994345672	-25.20759230136007	4.49264406545411
C	35.89244072112428	-23.45385340174841	4.78973471969553
H	34.87707022912029	-23.22750009098570	4.44439808384010
H	35.95643694091705	-23.19337373961188	5.85268564127637
H	36.59246002467627	-22.81551628952798	4.23748938867918

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B3LYP Scan/Thiolate IPC Model/BSS/350 degrees Constrained Optimization

C	30.38109106750911	-24.80660955174901	2.71331228822017
C	36.32968814273502	-24.54791330599460	10.66749768748688
C	39.31323436675128	-30.06176675336721	5.77379222258062
C	33.22866941447494	-28.84697983483262	0.72364430187378
N	33.20403450906854	-25.58896341266609	5.06130380023438
N	34.89732077646953	-25.52210380205912	7.33796947298001
N	34.73549393102361	-27.78411978555924	3.99256765519245
C	32.68951248830051	-26.84878467481082	3.02455079864355
C	33.10128820547551	-23.92940002920286	6.85563369384181
C	36.75691551308121	-26.66226662232071	8.45210505972963
C	36.80729189663337	-29.05187719969486	4.25648695465879

C	30.70821649198880	-22.79118194896034	5.24890970949702
C	33.91620193295425	-22.66135570819991	9.56525889638946
C	39.20005770263231	-28.54680318545702	8.65425790468796
C	36.07191095842788	-30.23482036880004	1.48349018133670
C	32.45345326914624	-25.83250128673911	3.94619965570541
C	34.13599212133958	-24.42660615003921	7.64322380825905
C	37.08986026557984	-27.56699626620343	7.44888426473416
C	35.66184468936228	-28.68563658713171	3.55733060488847
C	31.38844105430960	-24.84629361415059	3.82448771820350
C	34.53539919535995	-23.87050796510105	8.92740374472312
C	38.25640778276247	-28.43984281011429	7.49283991643208
C	35.27307205282965	-29.23302424852216	2.26536615123886
C	31.52614895370769	-23.99670447128198	4.88961370685942
C	35.54787656028337	-24.66644035256058	9.39256326150201
C	38.30079919615925	-29.07949186253217	6.28452844480113
C	34.07880419082527	-28.64635217062579	1.94323322180130
C	32.66150639456990	-24.48489304795879	5.65727589918596
C	35.76487019157435	-25.68917362767131	8.37957302460574
C	37.14417451116809	-28.61380801793469	5.53210025011394
C	33.77193249601354	-27.72365132281438	3.02850010295704
N	36.43155101661504	-27.70747715740326	6.26233279601206
Fe	34.77793159388296	-26.69460918680757	5.69442663519035
C	34.67121873863913	-31.40069833028275	6.14036161081792
C	33.67825377497802	-32.13594401585465	5.24775290854882
C	32.30260249405669	-27.36491488594096	7.30845446860685
C	33.52963054936411	-27.91228487573976	6.62719375499804
C	33.58852796261178	-29.37665816797796	6.77743707398936
O	32.86738324589039	-30.05173366435208	7.50913371395880
C	34.54723593326309	-29.98346655169937	6.01894465483719
H	29.89920624173014	-22.62488496335177	4.52942598389418
H	31.31809277223579	-21.87734914688692	5.27188585532666
H	30.24708488732544	-22.89121014540119	6.24129995543803
H	30.85753551324032	-24.64746044663246	1.73586127006725
H	29.81593495396400	-25.74622664584787	2.64191764037599
H	29.65436804168371	-23.99959357266530	2.85735258104177
H	33.10692985096393	-27.91585849456551	0.15276721843638
H	33.66745025446111	-29.58887307722409	0.04753191675892
H	32.21905890183879	-29.19540135764249	0.98257802412315
H	35.57889856650895	-30.49245787462081	0.53947760085452
H	37.07188261754983	-29.85170273817147	1.23739213548773
H	36.21792211091650	-31.16951746858690	2.04248120842275
H	34.40620957946325	-22.41299769120748	10.51319813786622
H	32.84853987183158	-22.81258148317331	9.77824354237260
H	33.98895142901358	-21.77741262967992	8.91665834104174
H	37.40436393163686	-24.42608924654819	10.47420492236933
H	36.22026216846135	-25.44087192246051	11.29884048168059
H	39.99790974808020	-29.27176650383945	8.45949842504354
H	39.68016501527538	-27.58437425467709	8.87991342098763
H	38.68382365024371	-28.86698210156834	9.57021215338659
H	38.85420147170534	-31.02451285774173	5.50882499148320
H	39.81662646598924	-29.68936013603836	4.87084027351946
H	40.08894550362426	-30.26492539184340	6.52025041170278
H	36.00343913131576	-23.68667345117276	11.26109849350634
H	33.75994804245995	-31.78276125877499	4.21618460901606
H	33.87122935369398	-33.21529132471595	5.26270031727758
H	32.65816625590065	-31.96334857699057	5.59501145533370
H	34.53887244150435	-31.69178494043992	7.18514108740117
H	35.69966995126696	-31.61032175595155	5.83656834384552
H	32.45797837104978	-26.36283882578325	7.70278243558162
H	31.48135731003142	-27.28573795387053	6.57902171421104
H	31.95078364169080	-28.02294199652848	8.10775126736160
H	32.00373141384711	-26.91967215783367	2.18526993147642
H	37.37415471033783	-26.66825315374864	9.3455532460505
H	37.47519540014246	-29.76432150121309	3.78121127677250
H	32.57711460739025	-23.05119691477628	7.22009397700142
S	36.31437897371870	-25.22231080127053	4.47968392407802
C	35.89870549827621	-23.46507502400000	4.79614109009682
H	34.88139284209656	-23.22235475919831	4.46803920633363

H 35.98224114332626 -23.21327603852486 5.85983259525244
H 36.59891673238934 -22.83204959371766 4.23803143884417

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B3LYP Scan/Hydroxide IPC Model/RKS/0 degrees Constrained Optimization

C 30.62609854822264 -24.78244147398106 2.31331079751440
C 35.59554000287882 -24.47200987300858 10.92574844254603
C 39.28502772079111 -29.82529819817738 6.36370760097021
C 33.80574931663983 -28.72458670577561 0.63256304310104
N 33.13774058977420 -25.56261757268173 4.99257279830023
N 34.54892497607929 -25.48156492201468 7.46573534956473
N 34.84016337097012 -27.70946414320477 4.09522190967239
C 32.90487677815133 -26.80740139990427 2.89805321309915
C 32.85185166356401 -23.87530711440090 6.74119912667147
C 36.28034561139603 -26.60234055499451 8.78456636290172
C 36.92613729788717 -28.88233180771394 4.58084418411143
C 30.65742020366854 -22.74869310849746 4.85372668084402
C 33.35575680695703 -22.57374452196656 9.51979622804280
C 38.76819451637779 -28.39651042828797 9.24094841890867
C 36.60034814834761 -30.00448556977856 1.70412681309835
C 32.53391509489505 -25.80635947971381 3.79291510984450
C 33.77522160133071 -24.37343848668520 7.66002297606849
C 36.75784418857537 -27.48577080489344 7.81897571169873
C 35.85927952318399 -28.54392014655862 3.75385408268089
C 31.49427494498887 -24.81691893604830 3.53688853979187
C 34.02680701891040 -23.80115546678055 8.97676189882228
C 37.95629343894363 -28.30393504055226 7.98241143126934
C 35.66148959064448 -29.06712107784341 2.40595945248729
C 31.50876071513574 -23.95855186304453 4.60349034681652
C 34.96568613141348 -24.60192461820854 9.57008460553061
C 38.17225320258568 -28.90648642032109 6.77414569294683
C 34.48846373366213 -28.52650627119582 1.95368411633743
C 32.54162174123594 -24.44778816672303 5.50789427051722
C 35.29034033996852 -25.64029548824546 8.60030011254070
C 37.08612808161394 -28.47298495848320 5.90083141078805
C 34.00643771661456 -27.65260557687539 3.01986457169260
N 36.24665647802857 -27.63292297693848 6.56554902889399
Fe 34.62605575742645 -26.67778034820324 5.82120064636937
C 34.51626889690001 -31.35711608336885 5.99714723808537
C 33.70275087798670 -31.96070157360897 4.85785565518772
C 32.13660211654306 -27.38410100432638 7.25053377578057
C 33.39173570546286 -27.85591006467111 6.55474619476058
C 33.38911805826455 -29.34610123008526 6.58732380847866
O 32.51406235475839 -30.04052844237435 7.09377533820352
O 34.46568367119443 -29.92993403658580 5.99101838329509
H 29.94074475833210 -22.58333897346033 4.04140361035976
H 31.26164076908243 -21.83529045850876 4.94801680191664
H 30.08003071995483 -22.84286602132742 5.78423998160610
H 31.21873934868746 -24.66662083301706 1.39495374573563
H 30.04360697988679 -25.70763004008464 2.19980743674828
H 29.91356306957801 -23.95078488408181 2.34868063826877
H 33.69274897181895 -27.77836811512109 0.08484505239094
H 34.36851259707435 -29.40870486500355 -0.01243989007581
H 32.79682602918714 -29.14381191469175 0.75255537738609
H 36.25401493243653 -30.23650918577514 0.69079485432710
H 37.60890234270034 -29.57691126715902 1.61586460275049
H 36.70615226104868 -30.95818041163130 2.24009979604876
H 33.71795643551883 -22.32922174527292 10.52462364180965
H 32.26570133376995 -22.69896516928302 9.58649879939667
H 33.53516763636045 -21.69553710234674 8.88354086690819
H 36.68311122381783 -24.32818793207966 10.85777993146606
H 35.43306570684363 -25.36919375928418 11.53937845385224
H 39.61557511271576 -29.08080943316083 9.12173192135025
H 39.17498918532159 -27.41993026538631 9.53973446296389
H 38.16925788644233 -28.76256807604054 10.08696280473078
H 38.90974093645380 -30.80381513119504 6.03225604594317
H 39.86550652819114 -29.40913614143395 5.52823580038012
H 39.98395235128188 -30.00754314518517 7.18794819390217

H	35.18686657655346	-23.61977592427015	11.47991524898620
H	34.01728413045284	-31.53899401089958	3.89978187521105
H	33.84012516591950	-33.04833688474184	4.82309021772160
H	32.64121938393700	-31.75110598995381	4.99879995582272
H	34.16377591789378	-31.73166247309304	6.96160298894542
H	35.57776838429525	-31.59211549987710	5.88617219149229
H	32.05720791074917	-26.30345571919504	7.30019766392354
H	31.24438612667074	-27.77419083819564	6.73986760119022
H	32.07866798508562	-27.78798764289834	8.27084036724044
H	32.33351029684277	-26.87657212287289	1.97669407629615
H	36.79131606736589	-26.60136655501026	9.74333244618399
H	37.68091088674868	-29.54897320155194	4.17278891030004
H	32.30155693403042	-22.98303429206788	7.02568658780351
O	35.87007772573244	-25.43595991780438	5.08858428959410
H	35.53490886324496	-24.54291468031442	5.25671217888779

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B3LYP Scan/Hydroxide IPC Model/RKS/10 degrees Constrained Optimization

C	30.61269390827226	-24.80302205127167	2.32527349872555
C	35.62180054031131	-24.43815352750527	10.91411094593512
C	39.26652617722515	-29.84884301102350	6.38485850928657
C	33.79600381956483	-28.74071895216334	0.64795513408023
N	33.12526821770111	-25.57630509429118	5.00561496144600
N	34.55093222225530	-25.47708266505560	7.47015827140990
N	34.82695772787689	-27.72639455014178	4.11205891611748
C	32.89100782731477	-26.82631371378053	2.91417574581911
C	32.84911345505538	-23.87663186048573	6.74384120148341
C	36.28491002312945	-26.59279675383119	8.78989866164460
C	36.91553778060103	-28.89604160883573	4.59742668054205
C	30.64868872641102	-22.75967983291372	4.85782716718193
C	33.37863543288453	-22.54637372736920	9.50394393670923
C	38.75939788571503	-28.40377722796320	9.25567092816414
C	36.59416272677910	-30.01377114864162	1.71823785290826
C	32.52017035769939	-25.82383789292173	3.80741939201319
C	33.78018334957385	-24.36571798003370	7.65976071264244
C	36.75593784574749	-27.48453364166366	7.82885448350991
C	35.84788417963965	-28.55913992262584	3.77058798765378
C	31.48080328279601	-24.83463509714269	3.54898215546563
C	34.04193368289955	-23.78168960901873	8.96916448914817
C	37.94942353747368	-28.30951444738559	7.99605644534206
C	35.65189636772751	-29.08100095508318	2.42185224590011
C	31.49708117649811	-23.97258278677894	4.61244509603806
C	34.98243955996705	-24.57965455631176	9.56403963487860
C	38.16178260212041	-28.91833853126297	6.79043175564405
C	34.47793829126825	-28.54203578949761	1.96940260910583
C	32.53103558889556	-24.45905345959907	5.51731571698261
C	35.29818554744357	-25.62781501184445	8.60192877594825
C	37.07860380016997	-28.48135352419773	5.91519401140757
C	33.99376382133688	-27.67004073869193	3.03578753410249
N	36.24378004431688	-27.63440644900960	6.57632625412681
Fe	34.61797775070163	-26.68446689188966	5.83103353884248
C	34.49196384264882	-31.36323593495104	5.99113919657630
C	33.79710065805378	-31.87118825871374	4.73314556931231
C	32.15548654880786	-27.39281890514055	7.31086712726419
C	33.38857636222345	-27.86147524002568	6.57456594664620
C	33.34140993176803	-29.34949164284542	6.51804922030331
O	32.37751753242184	-30.03926876004704	6.83324169322893
C	34.48659307584421	-29.93684383973699	6.07429752040260
H	29.93233574321595	-22.59604726292433	4.04487263871245
H	31.25533954137794	-21.84745787061799	4.94789495510018
H	30.07123170851593	-22.84823838651193	5.78884946648122
H	31.20596421962707	-24.69423490985195	1.40648067555859
H	30.02645812569297	-25.72639085338876	2.21639966545352
H	29.90359889061243	-23.96825297077622	2.35629127145356
H	33.68168725007652	-27.79448928458127	0.10058670183766
H	34.35994407954947	-29.42380403965634	0.00291129911249
H	32.78782881825867	-29.16167371242309	0.76785643393614
H	36.24626349987786	-30.24837459909713	0.70605868233468

H	37.59999575058816	-29.58049415221971	1.62713921236823
H	36.70680660761495	-30.96663426242304	2.25425271142546
H	33.74910713623078	-22.29192599021757	10.50328028127414
H	32.28869469119297	-22.66721034192745	9.58004818221448
H	33.55607474972499	-21.67582826775889	8.85670209146737
H	36.70961021604899	-24.30081424946246	10.83755274588888
H	35.45872698066716	-25.32757051402107	11.53885390628428
H	39.60089584282078	-29.09591870328999	9.14000772217507
H	39.17455391042640	-27.42961070136132	9.55095174243536
H	38.15661734754194	-28.76121338868832	10.10265928182705
H	38.88177343643205	-30.82365405157687	6.05342503463436
H	39.85439768551207	-29.44028955239716	5.55075357360922
H	39.96061457219530	-30.03747818732039	7.21175236495083
H	35.22106318216520	-23.57773112845551	11.46138917387351
H	34.22457680482462	-31.40204432462061	3.84361544061736
H	33.91346958387124	-32.95844115925575	4.64643885756637
H	32.73203313435977	-31.63905675156501	4.77062269088819
H	34.02206805066778	-31.78340451330543	6.88470712518635
H	35.55213047590966	-31.62787742278444	5.98487704756945
H	32.11280801933763	-26.31512320558506	7.42748425673815
H	31.25021397014546	-27.72221127997214	6.78232630121091
H	32.08794695761699	-27.85618874270357	8.30583167185462
H	32.31915122486441	-26.89707270129685	1.99326777083566
H	36.79866640051331	-26.58747630221950	9.74719057205733
H	37.66840654589697	-29.56550715515378	4.19053238422266
H	32.30062202230607	-22.98197186326376	7.02431191428764
O	35.86027069719805	-25.44614716952358	5.08886024651395
H	35.55396292138093	-24.55212101610916	5.30095728010315

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B3LYP Scan/Hydroxide IPC Model/RKS/20 degrees Constrained Optimization

C	30.59707595773749	-24.81905426398338	2.33855370611997
C	35.65721509536131	-24.40653935500021	10.89722303162513
C	39.24965568596117	-29.87259489917315	6.39672159784080
C	33.80823545754182	-28.72314676203782	0.64161901908528
N	33.11821992948900	-25.58274975172589	5.01342991547553
N	34.55378236917310	-25.47525526238332	7.47230996016954
N	34.81655166605071	-27.73977320820783	4.12141989676754
C	32.88770539226469	-26.82961258835043	2.91932202155879
C	32.84355321220398	-23.88148043434987	6.74983414711422
C	36.29519332746251	-26.58345040272268	8.78923013580590
C	36.90055323084776	-28.91622353086223	4.61041532617716
C	30.62675350467403	-22.77913371804922	4.87384674771843
C	33.39933893265137	-22.52763885212367	9.49273379972039
C	38.76392756861584	-28.40158792323794	9.25781760134942
C	36.59860833021856	-30.00541834301785	1.71697564594571
C	32.51288498515821	-25.83147822599180	3.81563635693930
C	33.78402225824725	-24.36246593534064	7.66035312024204
C	36.75642187260343	-27.48594633655945	7.83373230873162
C	35.83793420961735	-28.57237117915443	3.77991519886655
C	31.46794369178505	-24.84720020618485	3.56034441037357
C	34.05733956531517	-23.76782930402485	8.96256814394171
C	37.94689253837977	-28.31517362540679	8.00216659384133
C	35.65073668200215	-29.08153683515987	2.42505822544247
C	31.48139292195706	-23.98687698344333	4.62509508007470
C	35.00372001880429	-24.56056747967085	9.55524061226541
C	38.15051341266385	-28.93483127281623	6.80070620105614
C	34.48069652023678	-28.53684787808784	1.96955827030101
C	32.52017326583836	-24.46884273060595	5.52709360058745
C	35.31022100459296	-25.61703756243455	8.59931339716518
C	37.06598985960721	-28.49854999059127	5.92672141610212
C	33.99033896605282	-27.67368077769683	3.03992223791412
N	36.23764958945321	-27.64310633727191	6.58477614689513
Fe	34.61177815629309	-26.69066783467867	5.83835404998982
C	34.41368984281215	-31.38969888666293	6.03741513736641
C	33.89799592269476	-31.84293645170816	4.67693230235782
C	32.16450805581142	-27.39693666589643	7.35133720929503
C	33.37723924074089	-27.86164730570032	6.57899982455905

C	33.27685217653205	-29.34002678481819	6.43001767659918
O	32.24373600861767	-29.99029920386365	6.54095763207534
O	34.45597619256798	-29.96508948312322	6.16192964778901
H	29.90708468602069	-22.61922966891734	4.06307038969218
H	31.22825264046162	-21.86336771336152	4.96267483089780
H	30.05252588372849	-22.87167299474516	5.80648698106268
H	31.18779109096422	-24.70582775184699	1.41862647617960
H	30.01603351864372	-25.74569582269383	2.22996856007002
H	29.88334940598300	-23.98833644868258	2.37202879559398
H	33.69294561720793	-27.77111067232527	0.10479283101683
H	34.37956250897589	-29.39598811744857	-0.00769232774199
H	32.80143590548924	-29.15055097408462	0.75013457636584
H	36.26344382100243	-30.21927526130192	0.69596739707204
H	37.60694818008224	-29.57408638721502	1.64776679197382
H	36.70122113280346	-30.96941931595325	2.23506131649531
H	33.77702572987276	-22.26622282574560	10.48757523706452
H	32.30978280373569	-22.64638312105368	9.57722445421530
H	33.57336086592598	-21.66212841361617	8.83785126308494
H	36.74381078457895	-24.26728507530548	10.80777297922316
H	35.50325891293051	-25.29110497422680	11.53113091281167
H	39.60170842544701	-29.09845790803001	9.14335386503938
H	39.18541405370578	-27.42666224406782	9.54153607722130
H	38.16502023124849	-28.74842643949031	10.11193564680194
H	38.85890516886158	-30.84617660678057	6.06885104941588
H	39.83873999932096	-29.47010604296376	5.56045768861653
H	39.94401517898120	-30.06229696919755	7.22318559794899
H	35.26034412015711	-23.54256626909612	11.44173586701844
H	34.47482973826765	-31.38018807110114	3.87331865818296
H	33.97879951348509	-32.93302600391960	4.58461725236525
H	32.85164083795585	-31.56028814964337	4.55809783024224
H	33.79443436303939	-31.80553430074155	6.83739699369056
H	35.44983613807549	-31.70293713025995	6.18687897858857
H	32.14914356684506	-26.32478354507183	7.51591592126017
H	31.24813097348123	-27.68518466362675	6.81969484002062
H	32.09961802172530	-27.89999906873148	8.32810643443061
H	32.31811976365020	-26.89722249630127	1.99678950552999
H	36.81535642073226	-26.57106403948826	9.74302108025489
H	37.65084987258901	-29.58946318648293	4.20502290592498
H	32.29415063301096	-22.98738525969596	7.03034866722261
O	35.85663430562953	-25.45958425503008	5.08713042663708
H	35.58047457074598	-24.56568381963727	5.33750079326401

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B3LYP Scan/Hydroxide IPC Model/RKS/30 degrees Constrained Optimization

C	30.61290497371590	-24.74059982851951	2.31548120755189
C	35.64333729648342	-24.45275920614788	10.89747142571426
C	39.20850279785416	-29.90697426020846	6.34904292584758
C	33.77830674209158	-28.67097490324635	0.60165753530583
N	33.11114362400960	-25.55624430527389	4.99686814705970
N	34.54410783541231	-25.47815533487087	7.45795155664849
N	34.78930133205137	-27.72930360439481	4.09235931287860
C	32.88025894691063	-26.77911730038274	2.88837823148225
C	32.83474884882604	-23.87585530315109	6.75356630483457
C	36.28887719641453	-26.59866367855230	8.76031169541115
C	36.85857256143533	-28.93276520807460	4.57634323945004
C	30.63588151491241	-22.73679669686147	4.87949853493611
C	33.37881889847681	-22.56313689317563	9.51901166344800
C	38.74993898665627	-28.43155928762452	9.21320897697554
C	36.53559795305096	-30.01612502992927	1.68115166758846
C	32.51128665461761	-25.78591501728710	3.79259207174718
C	33.77207080816220	-24.36982172347641	7.66036844392911
C	36.74619184155303	-27.49499806304136	7.79722696390091
C	35.79749596483502	-28.57751336206275	3.74825002912913
C	31.47488934034328	-24.79102588749575	3.54278854185597
C	34.04266325987014	-23.79231577965291	8.97092968428367
C	37.92951237198597	-28.33558435504736	7.96056786257103
C	35.60513416239648	-29.07574499576910	2.39020865734092
C	31.48587160814632	-23.94541898637116	4.61918272476051

C	34.99201569301742	-24.58949362176167	9.55260721010547
C	38.12181336377618	-28.95710637513926	6.75825684421925
C	34.44836581939101	-28.50535135772966	1.93342236494704
C	32.51634462250134	-24.44521241537359	5.52099099420726
C	35.30187860919391	-25.63206261988914	8.58252629701712
C	37.03840554826611	-28.50886380510140	5.88887316588354
C	33.96876014992818	-27.64115114647060	3.00745554350221
N	36.22308232934650	-27.64370191861258	6.54943437895063
Fe	34.59796764757383	-26.68122117300372	5.81499717134654
C	34.42415466975982	-31.40296310028433	6.29285428963640
C	34.20915808402783	-31.90757517652934	4.87169817666807
C	32.13825985572728	-27.39202775442451	7.30718866452259
C	33.36428354641418	-27.85021791808140	6.55206449052667
C	33.26927727082283	-29.32757286634876	6.39050604426774
O	32.22286632519731	-29.95742567277147	6.30622227803229
O	34.46808125400344	-29.97332336964643	6.37051872740899
H	29.91933136080377	-22.56391273722427	4.06860651606779
H	31.24090453279986	-21.82469123763659	4.98134368430681
H	30.05830655070894	-22.83814244694367	5.80916755223581
H	31.21065953713257	-24.61493350559908	1.40170330202997
H	30.02959748796120	-25.66339916432967	2.18815890642842
H	29.90175843865407	-23.90800805007378	2.35689035764678
H	33.67750475624981	-27.71266087331247	0.07316552375745
H	34.34329861471803	-29.34516543291848	-0.05174440922918
H	32.76551021924057	-29.08604687809738	0.70265328503919
H	36.20758766787593	-30.20627442826424	0.65313054858385
H	37.55645435050544	-29.61267432954557	1.63019881365977
H	36.60481554665074	-30.99045683609369	2.18588651549054
H	33.75521414023769	-22.31469411905906	10.51766960308213
H	32.28980095074524	-22.68833767305622	9.60162533785013
H	33.54858718179057	-21.68718982705856	8.87700715074788
H	36.72979067257313	-24.31027013438770	10.81156295561846
H	35.49034132757929	-25.34647419406177	11.51872074128066
H	39.58286157588930	-29.13343091742104	9.09371096678310
H	39.17853677204970	-27.46034787470310	9.49895017006779
H	38.15156778631903	-28.77751297277904	10.06812534209806
H	38.80483174732981	-30.87568051164185	6.02238514976995
H	39.79838070310424	-29.51089523539501	5.51025279187277
H	39.90443981833034	-30.10519836076033	7.17220771157100
H	35.24395846979353	-23.59728803967660	11.45350080683453
H	34.96328332480543	-31.49249140876741	4.20039652289833
H	34.27717059880366	-33.00206065149406	4.84416415800854
H	33.22414542061478	-31.61155406555191	4.50991544755743
H	33.63661528616876	-31.77627704169825	6.95342941471975
H	35.39567680542253	-31.72209276131587	6.67817330821273
H	32.08589711345891	-26.31457586465870	7.42308105271764
H	31.23301005209387	-27.74101205217020	6.79484322315123
H	32.10066214524420	-27.84734639525766	8.30982550769271
H	32.31511717589947	-26.83040176148957	1.96203972329864
H	36.81044032149907	-26.59535033865318	9.71345952726842
H	37.59819502442743	-29.61723272786693	4.16993089439112
H	32.28583052109966	-22.98461985733832	7.04400835727487
O	35.84973327148569	-25.45173420160627	5.06954229300137
H	35.56706842477482	-24.55695237030704	5.30921209832082

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B3LYP Scan/Hydroxide IPC Model/RKS/40 degrees Constrained Optimization

C	30.61595698337666	-24.70328934131293	2.31555896213084
C	35.67338912437013	-24.44322379799746	10.88465812215089
C	39.18354775540192	-29.93119849864448	6.33394887236905
C	33.76228810571448	-28.64196137060391	0.58839141428130
N	33.10463302780847	-25.54341436099332	4.99841706891664
N	34.53823721554348	-25.48044418023475	7.45982962899320
N	34.77606673129739	-27.72137826568104	4.08419229619034
C	32.88002781302144	-26.74745316470458	2.87822604251365
C	32.81970235543073	-23.88092601278769	6.77027924175672
C	36.30003661042228	-26.59288731795998	8.74627509342870
C	36.82878844153247	-28.95152221808647	4.57030327575179

C	30.62067227847088	-22.73040329180719	4.90353338202709
C	33.38151316591734	-22.56857555325471	9.53122837438122
C	38.75932484554121	-28.42846407268255	9.18871184169264
C	36.49039597882033	-30.03684571540939	1.67791918006105
C	32.51006430754789	-25.76095183288117	3.78941977629914
C	33.76315665892172	-24.37533686043019	7.67025912140513
C	36.74725167323077	-27.49397098307211	7.78340841159019
C	35.77250389020996	-28.58390507823684	3.74109448984763
C	31.47261889723334	-24.76553027282155	3.54597928973743
C	34.04437749958250	-23.79589172466319	8.97761977222453
C	37.92752427940692	-28.33939439798042	7.94302748537179
C	35.57606817847864	-29.07803707896784	2.38231289291435
C	31.47574585424434	-23.93306813545612	4.63255929110740
C	35.00510692806978	-24.58699918048037	9.54883012818858
C	38.10562748867670	-28.97214617499730	6.74454781878420
C	34.43041048097670	-28.48845492368683	1.92253080211347
C	32.50431531456447	-24.44012025589317	5.53244521811948
C	35.30862551510661	-25.62929299861679	8.57644520822285
C	37.01803483231581	-28.52335890319059	5.88048608072631
C	33.95976440862925	-27.61970877142842	2.99679012935682
N	36.21342571031391	-27.64788078667321	6.54039620548205
Fe	34.59071491163553	-26.67633194877397	5.81113748564562
C	34.32430452734620	-31.43342673120271	6.40041096776583
C	34.46025646800291	-31.93401344560348	4.96886074128251
C	32.11683285389700	-27.41434205832341	7.27538216650390
C	33.35220157610425	-27.85049835612549	6.52329521435876
C	33.24451007877314	-29.31590055247896	6.28411686655641
O	32.21546985730213	-29.89800882343486	5.97501703775524
C	34.40115037278320	-30.00414886261623	6.49655832108073
H	29.90448034709844	-22.55247584123993	4.09338982735829
H	31.22168331024070	-21.81674771176984	5.01517413746273
H	30.04218347162568	-22.84317798480657	5.83133167225774
H	31.21756772635747	-24.56698156493916	1.40584756276242
H	30.03474457112367	-25.62562341630229	2.17586734452653
H	29.90333932912283	-23.87224133251799	2.36270816757798
H	33.67711094141902	-27.68122596225938	0.06151938655695
H	34.31977919384065	-29.32289185096372	-0.06445229035549
H	32.74332423275373	-29.04252870039126	0.68550190520208
H	36.16778138254998	-30.21530417240170	0.64605935960080
H	37.52119804145392	-29.65817163131842	1.63787696530774
H	36.53057036350432	-31.01417760101343	2.17998757868452
H	33.76834168965526	-22.31668791063115	10.52504458481390
H	32.29398783620272	-22.69799221792627	9.62654668960651
H	33.54019598223968	-21.69304137033201	8.88582889078534
H	36.75776062413824	-24.29476987674498	10.78377428097885
H	35.53407121959292	-25.33598042002979	11.51053498364633
H	39.58753777426607	-29.13563938163390	9.06772634241549
H	39.19563811678555	-27.45689672538152	9.46135078956324
H	38.16757999068311	-28.76335521422123	10.05258310458434
H	38.77219575746857	-30.90136248692206	6.02143696811337
H	39.76681703078719	-29.54642813670477	5.48533108616019
H	39.88702508197904	-30.12422875632851	7.15197921205999
H	35.27664823134724	-23.58842168338905	11.44366718372156
H	35.38644115863659	-31.56842830500038	4.52188000016491
H	34.47090122279746	-33.03079744108808	4.95244851645336
H	33.62342533818961	-31.58479510806492	4.36292476408734
H	33.38035103528103	-31.77239227817330	6.83525766007783
H	35.15232990096150	-31.78939991276592	7.01862659842017
H	32.06968908055757	-26.34125782287005	7.43147012090611
H	31.21975921462173	-27.73955940493743	6.73367389428652
H	32.06377829633098	-27.90590796547717	8.26080479956807
H	32.31798269994174	-26.78930582129903	1.94953477846588
H	36.83108898967338	-26.58551863101045	9.69417451833665
H	37.56195740818703	-29.64274819346145	4.16354262780968
H	32.26822516040463	-22.99360227592809	7.06786330949598
O	35.84224963702886	-25.44533243472792	5.06476223221790
H	35.56263161912878	-24.55192273483072	5.31295162523265

B3LYP Scan/Hydroxide IPC Model/RKS/50 degrees Constrained Optimization

C	30.62343697737205	-24.65780851881369	2.30350536317818
C	35.67402058236920	-24.45624011993566	10.87874658177060
C	39.14844698904606	-29.96584708862096	6.31724958067841
C	33.74345510858755	-28.61581033645389	0.56853835080138
N	33.10258652854260	-25.52306637516547	4.98738392458288
N	34.53486610756202	-25.47629437459752	7.44981664634762
N	34.77628675085658	-27.69472926515157	4.05813961039486
C	32.88529085291581	-26.70748875661771	2.85539615411078
C	32.80575436056616	-23.88135686604001	6.77662375456875
C	36.30312348050207	-26.59100584378584	8.72548588086784
C	36.81151978603531	-28.95183099259804	4.54748006016493
C	30.60928055143205	-22.71732478739661	4.91560960648121
C	33.36543151933721	-22.58738801820362	9.54639151771462
C	38.74325895922521	-28.45100059002401	9.16855662301051
C	36.45148317383935	-30.04740048857298	1.66035288163943
C	32.51339904728827	-25.72826645696432	3.77364109181132
C	33.75309192585564	-24.37806472921235	7.67113117596263
C	36.74630061385184	-27.49078501277079	7.75979955534403
C	35.76045022546542	-28.57204737584009	3.71678806835858
C	31.47440027218996	-24.73272469886583	3.53713080482143
C	34.03429369615300	-23.80649628898587	8.98194033069719
C	37.91609816118199	-28.35029849082233	7.92074554795688
C	35.55500177837716	-29.06894459992668	2.36027422508957
C	31.46940823897166	-23.91393087811301	4.63396736690231
C	35.00253530719226	-24.59498026887184	9.54398516165373
C	38.08687577356952	-28.98708876161528	6.72336498414435
C	34.41764590529043	-28.46427332669713	1.89974122174601
C	32.49597854178467	-24.42833901485351	5.53198782890461
C	35.30933425437873	-25.62845963730267	8.56313683483043
C	37.00655822797329	-28.52425717448078	5.85741465796423
C	33.95930983716175	-27.58660197975117	2.97193862317872
N	36.21283621796365	-27.63788375736189	6.51558996275974
Fe	34.59287611524024	-26.65837048302609	5.79045494420725
C	34.29760369435854	-31.43968849259885	6.51650210199442
C	34.62326351987114	-31.95780272322159	5.12244951382337
C	32.12783993898764	-27.44441308465424	7.25332812510789
C	33.36567618447948	-27.84614436773491	6.48756650894296
C	33.28321779807808	-29.30725938538720	6.21907391949469
O	32.31335713858105	-29.86959914788093	5.73770135148409
O	34.38209078045224	-30.00946547543958	6.61675662402071
H	29.89421204675077	-22.53345566582508	4.10576850299762
H	31.20653399316398	-21.80255470775073	5.03813475878269
H	30.02907892854599	-22.84176977515074	5.84086654970380
H	31.22889072842735	-24.50679638406730	1.39866234136322
H	30.04705468297279	-25.58075012331900	2.14863909259133
H	29.90693265278289	-23.83054477089294	2.35814341499448
H	33.66499133796323	-27.65595508028158	0.03900697797514
H	34.29233773992600	-29.30378911206229	-0.08419322010942
H	32.72130583868464	-29.00673352952261	0.67111536959686
H	36.12559700410480	-30.22492190551976	0.62934040765234
H	37.48938439181588	-29.68875908159404	1.61842192371775
H	36.47245479988001	-31.02234731621034	2.16795433806111
H	33.75233671641650	-22.34121625859090	10.54162643537439
H	32.27873758401736	-22.72343366945293	9.64223962328482
H	33.51821647728391	-21.70577472692826	8.90783596313315
H	36.75714443993989	-24.30038572373201	10.77570536296082
H	35.54224447769756	-25.35412742721594	11.49894457548935
H	39.56716585552947	-29.16312621794949	9.04713978549730
H	39.18501013191824	-27.48364167757705	9.44724930734763
H	38.14639216611414	-28.78597997589025	10.02892895814359
H	38.72125466072622	-30.93403736490894	6.01970367551859
H	39.73150368551934	-29.60030123378106	5.46011401286645
H	39.85457496582168	-30.15896299601610	7.13301252153412
H	35.27368742289273	-23.60777389048427	11.44486681867460
H	35.60746829700676	-31.60936398988622	4.80355710739066
H	34.62171795481080	-33.05478637202314	5.12002556850371

H	33.88306122313949	-31.60627291771100	4.40310768614156
H	33.29687455866480	-31.76096313052483	6.81804184736315
H	35.02530784407979	-31.80177584325508	7.24715064714557
H	32.05241793448116	-26.37191267430703	7.40646546960590
H	31.23364071773094	-27.79693759333178	6.72301624990860
H	32.10634759728860	-27.93251948059536	8.24207688199592
H	32.32440630765689	-26.74246840995673	1.92569777847348
H	36.83515527805577	-26.58836206144128	9.67290382028453
H	37.53572401808115	-29.65312796008731	4.14191210371711
H	32.24938347628203	-22.99993924474270	7.08266625940533
O	35.84133540170092	-25.41740535633834	5.05293385669859
H	35.55944774323852	-24.52627489671890	5.30646505670102

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B3LYP Scan/Hydroxide IPC Model/RKS/60 degrees Constrained Optimization

C	30.64782152652337	-24.57106473839821	2.27241591958761
C	35.65240809100813	-24.52762671080822	10.87669278599924
C	39.12853776790320	-29.98312152542042	6.24395450666412
C	33.72560070220818	-28.54869677676269	0.50966568961546
N	33.10190634333539	-25.49632641439306	4.96001547249383
N	34.52737795001305	-25.48735238609280	7.42593999006245
N	34.76510085318187	-27.66767885677665	4.00746124981975
C	32.89296018077764	-26.64326246401423	2.80661203075612
C	32.79095629343868	-23.88998514430325	6.77931863136267
C	36.30149801384469	-26.61426562686067	8.68274549174083
C	36.77586564581299	-28.96521373328097	4.49401696650840
C	30.60959744599594	-22.68823179342207	4.92577413491351
C	33.32888668773780	-22.65297372298038	9.57928779919647
C	38.74345168421977	-28.47552159753911	9.10140498582199
C	36.39187017205305	-30.05243020104971	1.60716732588507
C	32.52190136116081	-25.67603078670465	3.73757622580991
C	33.73698767696789	-24.40008758515361	7.66758951473214
C	36.74204553297604	-27.50462335577834	7.70719242384537
C	35.73083555422275	-28.56507153314214	3.66501430499236
C	31.48699575714148	-24.67371189050274	3.51206986826176
C	34.01109311611925	-23.85280906597500	8.99029521538232
C	37.90894666412967	-28.36931108684852	7.85900859426552
C	35.51786845589019	-29.05338417886353	2.30644717739549
C	31.47242686649382	-23.87851092648899	4.62603331435207
C	34.98602090776984	-24.64339526768639	9.53729272901129
C	38.06906695682974	-29.00582951935968	6.65993601118018
C	34.39761508089438	-28.41954986489504	1.84423116165767
C	32.49139476371047	-24.41187900280825	5.52150140172180
C	35.30251420564267	-25.65478849179753	8.53656042494374
C	36.98498826933153	-28.53691887566681	5.80188446839036
C	33.95377073810874	-27.53844003248966	2.91973759416645
N	36.20206586107278	-27.64437460711762	6.46492344082867
Fe	34.58729795472598	-26.64750059897226	5.75085701322734
C	34.27276620210790	-31.42268612216490	6.78775376453189
C	34.84982707613139	-31.98924532243198	5.49837142734938
C	32.10441167395105	-27.46100192329034	7.17622629432733
C	33.36613573229923	-27.84233563071087	6.43987902380249
C	33.33467264834517	-29.31109334907857	6.21595860721919
O	32.47031576555688	-29.89387542447498	5.58563248151407
O	34.33821692219122	-29.98782895726142	6.84622626571681
H	29.89823234507163	-22.48999855490843	4.11603302499493
H	31.20483223568829	-21.77505080925975	5.06852047835170
H	30.02492609529110	-22.83086644617400	5.84558980617211
H	31.26167145045372	-24.39669842966874	1.37743744370567
H	30.07546613471422	-25.49135475043803	2.08943496458544
H	29.92862017464665	-23.74709213223401	2.33996820816530
H	33.67062219682683	-27.58420157687513	-0.01447048006855
H	34.26188856459554	-29.24467286937557	-0.14501616650179
H	32.69465157552978	-28.91748320348811	0.60604367555759
H	36.06263924275739	-30.22258599148808	0.57594695537965
H	37.43811798688576	-29.71863211796591	1.56556810052296
H	36.38942751652927	-31.02705906897755	2.11574734911365
H	33.71148179470762	-22.42416571963321	10.58031939378354

H	32.24346014852505	-22.80226150743728	9.67005200546770
H	33.47351663122780	-21.75629849281744	8.96007792537029
H	36.73480976631920	-24.36269527055082	10.78046161500696
H	35.52464848809153	-25.43920538882189	11.47746787043343
H	39.56570150211294	-29.18829095675871	8.97276488029959
H	39.18779351021192	-27.50971353923159	9.38110879460157
H	38.15099820308149	-28.81305246636512	9.96384119133684
H	38.70313170150813	-30.95376935506732	5.95155039350619
H	39.70153497275362	-29.61626685076095	5.38069118983808
H	39.84352904075035	-30.17316160211493	7.05268695071746
H	35.24461888636095	-23.69378591717521	11.45902244490508
H	35.87362747463614	-31.64068602852073	5.34991540226469
H	34.85308938064026	-33.08540277966156	5.53749985914826
H	34.25154802867618	-31.67158520929526	4.64401005098856
H	33.23305119554140	-31.73796483664184	6.91062440630211
H	34.85171782819479	-31.75262637510139	7.65400381377404
H	31.99488838607073	-26.38768827297336	7.30290459490815
H	31.22953604259719	-27.84909950094605	6.63683470984839
H	32.08102559281060	-27.92815346158441	8.17499871583168
H	32.33760569880944	-26.65997213356146	1.87304301737428
H	36.83556970451812	-26.62203354163293	9.62897575655364
H	37.48615078279127	-29.67970073090825	4.08696171322237
H	32.22946896280992	-23.01718228764926	7.10035831122239
O	35.84159884924154	-25.40113206475506	5.03046290825988
H	35.53779681019674	-24.51040124741418	5.25882189400301

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B3LYP Scan/Hydroxide IPC Model/RKS/70 degrees Constrained Optimization

C	30.66960574650051	-24.60314224238087	2.25891800372944
C	35.60903408227671	-24.51441565908077	10.90195944796419
C	39.12834531322306	-29.99101953955790	6.32559329128749
C	33.85475879490671	-28.49418330590010	0.49135834815138
N	33.10710521053200	-25.50928423810266	4.96747599343817
N	34.51070732917167	-25.49505360313537	7.44797635832166
N	34.80647887542337	-27.65850193665884	4.02528317019174
C	32.95141230704240	-26.63420657154138	2.79860440550655
C	32.75195549775525	-23.92314004812163	6.79496198208386
C	36.28488864032982	-26.60460629231665	8.72099140896146
C	36.80623407922423	-28.96223374706552	4.54214428978134
C	30.55818883594896	-22.75325828058183	4.93289092467331
C	33.26760220275577	-22.67141047748109	9.59144670410690
C	38.72268918830105	-28.46523622151400	9.16995448382134
C	36.49848353057786	-30.00503934012319	1.63177120990332
C	32.54790165900982	-25.68610912824601	3.73530818966111
C	33.70440008428470	-24.41743479068326	7.68532938721158
C	36.73452024438320	-27.49907970018261	7.75359350449970
C	35.78139114390137	-28.55033939883446	3.69416492386159
C	31.49541025684781	-24.70247263073455	3.50785156980522
C	33.96592909496928	-23.86476415811984	9.00806026833461
C	37.89881131782241	-28.36427828201593	7.91999215173730
C	35.60248265310099	-29.02087704728463	2.32458469502666
C	31.44964029459878	-23.92159019416698	4.63095181460216
C	34.94853173423315	-24.64212902529942	9.56067135652610
C	38.06790879700385	-29.00836209443592	6.72618469721999
C	34.49193722706882	-28.38333177082205	1.84448569421377
C	32.46893039498256	-24.44409864375509	5.53304465652466
C	35.28096642104529	-25.65186462978345	8.56397719870026
C	36.99390033986419	-28.54071650702194	5.85529110289142
C	34.01964192110142	-27.51894973644292	2.92128483698292
N	36.20519536436598	-27.64393001077906	6.50678439702878
Fe	34.59561896120860	-26.64846674517403	5.76956546850391
C	34.05789262937578	-31.49144822087952	6.56717210702078
C	34.80235474237855	-31.97986105339563	5.33332138271369
C	32.14875302445983	-27.51592098356706	7.24392472900411
C	33.36677111742208	-27.85318227322651	6.41919833039681
C	33.29020157156579	-29.29267602447732	6.06362709054930
O	32.48794131459838	-29.76980143644485	5.28377800013876
O	34.17364859873284	-30.07057889821024	6.75710601196321

H	29.85071815773555	-22.56335514783826	4.11772658881731
H	31.13164683206745	-21.82847324116299	5.08967256978436
H	29.96779546889257	-22.91709841917820	5.84551394594863
H	31.29058856987895	-24.40369867476087	1.37409501746645
H	30.12078743329722	-25.53379493664890	2.05739964254258
H	29.93125165927482	-23.79635740505892	2.32751414937241
H	33.81592457357353	-27.52314779258815	-0.02201318028314
H	34.40630783086367	-29.18367169893640	-0.15753897595812
H	32.82103037995529	-28.86182030600259	0.55661651327557
H	36.20322207813417	-30.15114284401602	0.58666916503121
H	37.54528480290534	-29.67072660014171	1.63201687094111
H	36.47988713074856	-30.99130126845250	2.11719224052431
H	33.64283498988364	-22.43627762582879	10.59378500033890
H	32.18348010783772	-22.83249547624129	9.67742144081874
H	33.40523309997054	-21.77462805834349	8.97083516600083
H	36.68908332324988	-24.33306075178726	10.80863688125566
H	35.49342250441590	-25.42693223147782	11.50375392313375
H	39.54518949454334	-29.17945447241992	9.05138962684761
H	39.16577495978976	-27.49852105027409	9.44854470581896
H	38.12274924217169	-28.79803392632505	10.02905925362403
H	38.70222343008159	-30.96084361570573	6.03158285591621
H	39.71276291252072	-29.62954876262910	5.46769098133222
H	39.83315265576108	-30.18104639511727	7.14319076825045
H	35.18686055917582	-23.68605193969220	11.48179175642973
H	35.85192922391616	-31.68177993137824	5.37259964175269
H	34.74918795846945	-33.07362171931566	5.27036117786315
H	34.36047612969109	-31.55533866985676	4.43136878489582
H	32.99956893808097	-31.75800335626058	6.50593479653812
H	34.48262199284476	-31.92091474193086	7.47812150230787
H	32.07873980369627	-26.45843299785750	7.48389674085946
H	31.23782643438378	-27.82112013598627	6.70891367703804
H	32.15475675365695	-28.08348193039124	8.18934617154309
H	32.41353786313744	-26.64662738388541	1.85481583775645
H	36.81228850249250	-26.60578335719294	9.67097319743729
H	37.52186486414551	-29.67663056006876	4.14449650498891
H	32.17374794687021	-23.06133861665986	7.11618536680735
O	35.84130606925994	-25.38948962211953	5.05388286651781
H	35.57095875833086	-24.50887977592397	5.35275902242357

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B3LYP Scan/Hydroxide IPC Model/RKS/80 degrees Constrained Optimization

C	30.70906939458791	-24.42022480655000	2.20811906076490
C	35.54503505833281	-24.72063252806238	10.90271492589036
C	39.06665468596694	-30.04949539581430	6.14483944623053
C	33.82688054959181	-28.32054171969425	0.34671142373863
N	33.10178863596112	-25.46119898524199	4.90921756748613
N	34.48238249504978	-25.54721669285594	7.39837888929093
N	34.77715071767062	-27.60266669108503	3.90680893389703
C	32.95181203844036	-26.50564661658184	2.69920526733669
C	32.73669852968274	-23.94350005231669	6.79344298709381
C	36.24469173420625	-26.71263364798975	8.63784627961078
C	36.73710261322129	-28.97241603573582	4.39962977969294
C	30.58632120814123	-22.67329347640561	4.94983498399158
C	33.21468909400368	-22.82387441328451	9.65213651853308
C	38.67144079092424	-28.59919904600163	9.03287938173168
C	36.40903744540091	-29.94591889953350	1.46902944942316
C	32.55422196773977	-25.58388322645051	3.66475482734079
C	33.67393493442123	-24.48223189042083	7.67436631038949
C	36.69147094488559	-27.57952567759406	7.64400358514631
C	35.72614972471324	-28.51514513216220	3.55948491685099
C	31.51761156498782	-24.57852402195163	3.46216285212225
C	33.92229359781493	-23.98777697229515	9.02265143621556
C	37.84546995873415	-28.46156860216002	7.78781997087134
C	35.54231102375036	-28.94729967013146	2.17752155555923
C	31.46757256239650	-23.84010775411242	4.61367277896859
C	34.90122702384747	-24.78696425377383	9.54912940529454
C	38.00784578341852	-29.07789800314481	6.57725776607715
C	34.45701448069386	-28.26386743297132	1.70630757045388

C	32.46913959997627	-24.40858875595430	5.50680805468165
C	35.24395993882540	-25.75242619931081	8.51232037333903
C	36.93753626732133	-28.57782218206240	5.72012739562455
C	34.00102328797928	-27.4148242220460	2.80325371695690
N	36.16252183507059	-27.68491913589672	6.39292005595784
Fe	34.57087466658693	-26.64469790646661	5.68244428830514
C	34.12744940353478	-31.38224959203115	7.14508673245320
C	35.28619429708999	-31.93282485038623	6.32860495236016
C	32.02582175527081	-27.54346565193790	6.96377087348884
C	33.34491356869119	-27.86389161104696	6.30502186599396
C	33.42304701060979	-29.33540850311238	6.13391248603630
O	32.88594105446960	-29.96834324346633	5.24780603328323
O	34.10878610295055	-29.94455806709639	7.15142068446693
H	29.88501489509344	-22.44918360373724	4.13805317457529
H	31.16814854800555	-21.76002893679522	5.13997805228324
H	29.98963440905193	-22.86137150279158	5.85359566797654
H	31.34187909165609	-24.18017306079553	1.34184042960064
H	30.16270488646818	-25.33978378476023	1.95562683967494
H	29.96999675473561	-23.61693322158300	2.30413128933172
H	33.82373887407631	-27.33665657478212	-0.14341432826682
H	34.36035414334064	-29.01201418408459	-0.31498130233804
H	32.78110083658480	-28.65542978258896	0.39556136045706
H	36.11782974066051	-30.05800762953905	0.41858521174658
H	37.46721111724526	-29.64998440221135	1.48490374358181
H	36.35041704824806	-30.94141317134563	1.93187137833013
H	33.57756339208908	-22.63423768986010	10.66856919118105
H	32.12999793198311	-22.99079209150831	9.71783990012130
H	33.35723389825722	-21.89894315195675	9.07542168187429
H	36.62719840094033	-24.54228392556932	10.83080451987603
H	35.41649582114578	-25.65766759516609	11.46278689096082
H	39.48395655281703	-29.32192172454334	8.89799948103085
H	39.12805026897468	-27.64424632765439	9.32941403623213
H	38.06888895002252	-28.9409999849168	9.88645353373137
H	38.63872294442167	-31.00661312688573	5.81501084355380
H	39.65322184026210	-29.65792834973319	5.30180843572266
H	39.76918257660780	-30.27022362266668	6.95666568027336
H	35.12018053772091	-23.91533902319382	11.51239109861250
H	36.23381644936848	-31.52665088846170	6.68877147910701
H	35.31797666391380	-33.02655249442991	6.40415596706407
H	35.17426503191663	-31.65767876571207	5.27895270924209
H	33.17328311312258	-31.75086600628053	6.76103117046918
H	34.22150956430374	-31.66022446204121	8.19832477278189
H	31.87495702606985	-26.47743646777735	7.11285445001007
H	31.19888300916737	-27.93340655219753	6.35080885508995
H	31.94787538105901	-28.04682784924704	7.94108416244187
H	32.42288609618095	-26.47691016449090	1.75064507121966
H	36.76731430931638	-26.75026340768916	9.58972475107464
H	37.43315935897345	-29.69835596237309	3.98895730786025
H	32.15974197190054	-23.09217123742750	7.14344535449458
O	35.83774972094596	-25.37974402899185	5.01685324633382
H	35.49696547439098	-24.49338525274189	5.20683429273756

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B3LYP Scan/Hydroxide IPC Model/RKS/90 degrees Constrained Optimization

C	30.71987643116272	-24.37127743123303	2.19140067108128
C	35.52479594242516	-24.77994199745999	10.89791236247580
C	39.03797430647246	-30.08139275430548	6.09665572900597
C	33.82621422046438	-28.26785660662973	0.30124180854134
N	33.09770034467105	-25.45241524481560	4.89012444529384
N	34.47378415918674	-25.56501356182774	7.38040276214018
N	34.77634824082030	-27.58106330799290	3.86739966675609
C	32.95582156066870	-26.46866574000308	2.66663990581716
C	32.72554945583157	-23.95802227870917	6.79183212522442
C	36.23578402481528	-26.74156173942383	8.60991939536640
C	36.72493646638587	-28.96903748679403	4.35335043356611
C	30.58671972287005	-22.66070806704055	4.95515929161591
C	33.19324184670505	-22.87349185347550	9.66506595927578
C	38.65643373206508	-28.63834306260370	8.99205492797312

C	36.39398167007935	-29.92044466701958	1.41693500798809
C	32.55560106795116	-25.55791330501883	3.64170236217711
C	33.66151508708278	-24.50602394518645	7.66815341132808
C	36.68270584554905	-27.59962764418275	7.60862154301359
C	35.71933752656158	-28.49723505830251	3.51517993044905
C	31.52127332083602	-24.54874740596692	3.44743070314474
C	33.90550330346181	-24.02759153940249	9.02287455167882
C	37.83217564924055	-28.48837199498650	7.74712958406542
C	35.53495946262953	-28.91849856471728	2.12979920116265
C	31.46652275438313	-23.82558137687455	4.60846407606610
C	34.88566922257585	-24.83037415237436	9.54146595756313
C	37.99155250377184	-29.09849181236692	6.53268624477601
C	34.45536419305793	-28.22460948490643	1.66173316454592
C	32.46302020265000	-24.40691798795808	5.49854474366101
C	35.23353912240879	-25.78175984761893	8.49343594027039
C	36.92561625371107	-28.58647210294389	5.67759018835461
C	34.00260529837399	-27.38107431629626	2.76449921629754
N	36.15465578851648	-27.69375506509138	6.35590822638853
Fe	34.56636989563900	-26.64363560197232	5.65156962042124
C	34.10818146819928	-31.34870248486692	7.28309793637800
C	35.38582019663897	-31.86406626993282	6.63860228182062
C	32.02941760044730	-27.57603800324505	6.93111258209589
C	33.34905856129566	-27.87516095453073	6.26511199144168
C	33.48464682997342	-29.34665149642539	6.13285899237493
O	33.11521295424698	-30.01541146952965	5.19055302423252
O	34.03087359857337	-29.91341093949962	7.25691814813112
H	29.88612410767931	-22.42798491194842	4.14519917916163
H	31.16987411528644	-21.75006965172668	5.15386590821405
H	29.98941330649163	-22.85611073301468	5.85692618683314
H	31.35688931881663	-24.11301759208720	1.33343328999585
H	30.17872316664567	-25.28818086549416	1.91889299389135
H	29.97696456995662	-23.57277381863152	2.29728290957736
H	33.83182161256452	-27.28118448927390	-0.18335104888307
H	34.35433896307337	-28.96012884799548	-0.36386866459414
H	32.77753090178915	-28.59406882672311	0.34708688910558
H	36.10574542414015	-30.02138410425249	0.36452627558328
H	37.45518442294623	-29.63607484981287	1.43914247692745
H	36.32238336087946	-30.91857360851704	1.87210409285086
H	33.55133792095077	-22.69690968081844	10.68554132076203
H	32.10856665859725	-23.04296889500248	9.72383009673266
H	33.33670723768477	-21.94051444989218	9.10165832947760
H	36.60726941714105	-24.60128448232183	10.83193733633130
H	35.39381041655624	-25.72331347485530	11.44670682198669
H	39.46569839574911	-29.36392347068401	8.85301664960831
H	39.11708925998594	-27.68745719248365	9.29524063035527
H	38.05167356829525	-28.98296890654485	9.84288141265105
H	38.59646845552320	-31.03615679243342	5.77771485576050
H	39.62011799379231	-29.70086582085565	5.24570947548986
H	39.74584882699410	-30.30377439681642	6.90340748736759
H	35.09814947972080	-23.98152987170867	11.51536218225893
H	36.26154117696183	-31.41051230991646	7.10796934073936
H	35.45078122272039	-32.95381573081493	6.74488624816733
H	35.40197603399051	-31.61434080986367	5.57703431644282
H	33.22857410228718	-31.76379982370091	6.78517079478737
H	34.07319394835985	-31.60593066084723	8.34531588320539
H	31.85726423307080	-26.51135742717991	7.06783383057916
H	31.20185866591681	-27.98812060668896	6.33204546036884
H	31.97354747734075	-28.06992416458532	7.91391582082828
H	32.42996367942101	-26.42855611418318	1.71676781571401
H	36.75667006156704	-26.78918599528763	9.56226740602599
H	37.41609391004329	-29.69708567033512	3.93822804620073
H	32.14649477609095	-23.11191840399013	7.15090781178083
O	35.83344075646925	-25.37146406428808	5.00153497646677
H	35.48470320010075	-24.48733018789292	5.18752283028780

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B3LYP Scan/Hydroxide IPC Model/RKS/100 degrees Constrained Optimization

C	30.70726637403389	-24.37945117885710	2.19196767006093
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C	35.52637718395499	-24.79757789192224	10.89031464332367
C	39.03219744048353	-30.09542004949127	6.07972254653379
C	33.84904234054672	-28.23683086396359	0.27590783633174
N	33.09917600652372	-25.45335486858006	4.88072889646868
N	34.47707377615428	-25.57161964748676	7.36982974334902
N	34.78436914867980	-27.57265073828286	3.85036847765708
C	32.96174056877786	-26.46063296010011	2.65305484895894
C	32.72422065393849	-23.96692363330780	6.78790235154266
C	36.23774449735527	-26.75245188500657	8.59792974650412
C	36.73244027352909	-28.96267542214201	4.33331764949854
C	30.56880965976384	-22.68012542336083	4.96221423415657
C	33.19320943343251	-22.88917062704683	9.66354097615118
C	38.65824522964434	-28.65136667638299	8.97584213239712
C	36.41843538686253	-29.88873409422569	1.38915329684823
C	32.55577664958592	-25.55757567270961	3.63281977061992
C	33.66372857539489	-24.51407452010900	7.66099566378802
C	36.68353687096617	-27.60971021379098	7.59544528476832
C	35.73088132294163	-28.48358858989524	3.49489454544260
C	31.51384786803879	-24.55510315168299	3.44495709603637
C	33.90732085533945	-24.03973993433519	9.01710761942894
C	37.83234446199327	-28.49961483455051	7.73207765200663
C	35.55313438728641	-28.89495427880284	2.10573684494720
C	31.45686885936323	-23.83662807707701	4.60882539287615
C	34.88796407231345	-24.84351252303364	9.53336504031829
C	37.99095908336023	-29.10758365112430	6.51632874219264
C	34.47275877881887	-28.20166175679542	1.63910707102681
C	32.45968077503749	-24.41418749788131	5.49437307037330
C	35.23644779509892	-25.79151855087762	8.48270708499858
C	36.92712757963947	-28.59156481336553	5.66158228916644
C	34.01336822303323	-27.36791817049949	2.74679888340934
N	36.15517053964908	-27.70107770830523	6.34241733858810
Fe	34.56864642663378	-26.64474691519264	5.63700470929274
C	34.02228677763981	-31.35398547050826	7.30254317947952
C	35.36762046565509	-31.82328506640841	6.76887185379347
C	32.05817526255575	-27.57364441353853	6.96817390269717
C	33.34897915415108	-27.87530779841699	6.24926680703451
C	33.49078344470117	-29.34559295481507	6.11452767673030
O	33.24741015822635	-30.00939619084469	5.12962342748295
O	33.90542798247619	-29.92153136296161	7.29303682658560
H	29.86242544975170	-22.45185820410209	4.15601358980106
H	31.14489370432472	-21.76479229374122	5.16003241081923
H	29.97745623721558	-22.88255399400121	5.86634603726062
H	31.33790023912022	-24.10223701745696	1.33512087226598
H	30.18131624825313	-25.30287148027719	1.91198795844710
H	29.95106431642904	-23.59477439460190	2.30676550481121
H	33.85451563940335	-27.24694243681298	-0.20211970200756
H	34.38133660913338	-28.92351920456357	-0.39168574824425
H	32.80091132290417	-28.56571127649866	0.31520239735178
H	36.13268737697614	-29.98571406971269	0.33568558438324
H	37.47818256853198	-29.59914815531092	1.41478250692224
H	36.35076309022259	-30.88931356340542	1.83943017244203
H	33.55191753738288	-22.71505002303860	10.68421539064109
H	32.10900225709666	-23.06143665103031	9.72288509587935
H	33.33393824882464	-21.95414524377722	9.10290021140163
H	36.60882758682023	-24.61832115306880	10.82546112533926
H	35.39547204860627	-25.74295540104426	11.43564514597210
H	39.46935061998393	-29.37421104335605	8.83335155369559
H	39.11672755364224	-27.70008748322376	9.28103447561150
H	38.05594701910699	-29.00019316969200	9.82667868215949
H	38.58501707427505	-31.04989332737759	5.76782813312307
H	39.61112779762599	-29.72099019775265	5.22393595163254
H	39.74344781627359	-30.31650609212175	6.88383303201953
H	33.09916370828048	-24.00153105376700	11.51039755680718
H	36.18509373506589	-31.34088884602050	7.30942746846598
H	35.46138098595976	-32.91041899036409	6.88036830207496
H	35.46544529062442	-31.57054365283174	5.71257200578117
H	33.20402513553934	-31.78436772601167	6.71984887843415
H	33.89802139389607	-31.63149387599979	8.35291752601542

H	31.89155495426403	-26.50872158815969	7.10877778380743
H	31.20206568621662	-27.98567185900617	6.40942200619810
H	32.04811588520018	-28.06597026685801	7.95230566928521
H	32.43671554934607	-26.41781139272835	1.70283418510929
H	36.75865575682583	-26.80200673445403	9.55014064780580
H	37.42527409417969	-29.68735265181449	3.91511853847962
H	32.14263780576911	-23.12411050319646	7.15057577974391
O	35.83493075196004	-25.37089458577259	4.99071208532644
H	35.49629053938747	-24.48842064636911	5.20165414507134

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B3LYP Scan/Hydroxide IPC Model/RKS/110 degrees Constrained Optimization

C	30.69144865461907	-24.38656872441687	2.19693187277575
C	35.53294286573716	-24.81160724863740	10.88200675776809
C	39.03891209538103	-30.09399223800782	6.05555050494380
C	33.85496166204022	-28.21629076748913	0.25789273898238
N	33.10111281550183	-25.45176274856961	4.87304494533525
N	34.48010789928804	-25.57750610099668	7.36067683071093
N	34.79673654912763	-27.55641753995333	3.83122729038902
C	32.96305441212762	-26.45297665639811	2.64295241684969
C	32.72411301730573	-23.97339053672751	6.78605715838218
C	36.24188452154178	-26.76143101271150	8.58468438332288
C	36.74791304888743	-28.94445078296160	4.30730802545175
C	30.55416565993792	-22.69455977708777	4.97187034672866
C	33.19802607240156	-22.90092691649534	9.66228106760117
C	38.66410606560082	-28.65949773242969	8.95599277664897
C	36.43581643141567	-29.85795846932475	1.36086352907530
C	32.55395347829198	-25.55579446266652	3.62679390841889
C	33.66655063318098	-24.52096348626310	7.65554958768583
C	36.68935510221450	-27.61403652556021	7.57885338591841
C	35.74680374485619	-28.46119379212364	3.47111505680486
C	31.50501968828040	-24.55948170914899	3.44576113472143
C	33.91156940356915	-24.04992829980884	9.01242619080216
C	37.83882565199485	-28.50356361286314	7.71226715760830
C	35.56840402042322	-28.86873619516527	2.08093249009084
C	31.44828690368399	-23.84425529788699	4.61169573055782
C	34.89277080287291	-24.85492184194339	9.52580245762962
C	37.99925863100584	-29.10551598982647	6.49379832867083
C	34.48296030603983	-28.18054123298382	1.61906906527249
C	32.45769331803075	-24.41825939970236	5.49199783382441
C	35.24031261838058	-25.80030872628213	8.47247089802987
C	36.93779461517425	-28.58470042847468	5.63928662810089
C	34.02165502404271	-27.35280163159904	2.73068916396847
N	36.16284867377648	-27.69960179614502	6.32438211927769
Fe	34.57407173813761	-26.64322269183271	5.62219133570099
C	33.91930236169309	-31.37600088553873	7.30029901332092
C	35.33770182657486	-31.80597738513525	6.95407333917141
C	32.08603281948051	-27.58088960429178	6.97989244100141
C	33.35780191422939	-27.88250449164735	6.22759077763761
C	33.51684479283038	-29.35079861726208	6.08723871547025
O	33.42119742514257	-30.00458747906777	5.07127970969169
O	33.77385626917795	-29.94687203053520	7.30496274942261
H	29.84520358081692	-22.46653514958480	4.16785583545036
H	31.12525210741218	-21.77683006455512	5.17304046831096
H	29.96527168883073	-22.90437848727180	5.87595507039025
H	31.31638967704930	-24.10640733493975	1.33690850766549
H	30.16787105541484	-25.31208612189408	1.91932036321940
H	29.93249105104184	-23.60517341034791	2.31591981429256
H	33.85275485317046	-27.22538190975474	-0.21807764377286
H	34.38921749183076	-28.89825169164537	-0.41299172610464
H	32.80895382781079	-28.55169048766875	0.29974237092941
H	36.14770369714870	-29.95515263072065	0.30804573619057
H	37.49452539738471	-29.56438009661703	1.38413494263370
H	36.37275431652009	-30.85893342428257	1.81086810641326
H	33.55891107327516	-22.72796944220913	10.68239207250474
H	32.11409515528012	-23.07419842391855	9.72392465574820
H	33.33659177367067	-21.96493318196627	9.10274242554369
H	36.61534841907562	-24.63247762653970	10.81610668278386

H	35.40256297920557	-25.75788343505790	11.42590240805507
H	39.47323546215735	-29.38437876612495	8.81266229992219
H	39.12550135080377	-27.70988711804038	9.26219389216502
H	38.06125973692135	-29.00736614124477	9.80678969024991
H	38.59010737628758	-31.04691457532876	5.74138071996960
H	39.61909835064029	-29.71899140277150	5.20086171552198
H	39.74929653862986	-30.31820328684142	6.85952248214570
H	35.10672920695323	-24.01655980857124	11.50407791605638
H	36.05995017210623	-31.33568152254557	7.62530243477844
H	35.43580673650565	-32.89525040014644	7.03732580023803
H	35.58298248377488	-31.51020996139040	5.93348404949003
H	33.20410983516517	-31.80669707028972	6.59515912244590
H	33.65049049482966	-31.68451353732263	8.31455282543284
H	31.89815451669445	-26.51481021804754	7.07686223467471
H	31.21452482777893	-28.04094135419952	6.48602570681515
H	32.13634690164976	-28.02197849409015	7.98610585307369
H	32.43431877932478	-26.41146816203493	1.69472357877987
H	36.76217203551464	-26.81444763266261	9.53703737454450
H	37.44228979673313	-29.66533835349146	3.88517264837040
H	32.14047445337348	-23.13375648490752	7.15272845666995
O	35.83476083716945	-25.36319275837566	4.98036869406980
H	35.50051240604956	-24.48187549363714	5.20289833356632

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B3LYP Scan/Hydroxide IPC Model/RKS/120 degrees Constrained Optimization

C	30.67818077345241	-24.39130655003901	2.19729215672218
C	35.53806331163891	-24.84022019840750	10.87071451101068
C	39.05828024612333	-30.08150940809390	6.01305281804824
C	33.87350798940334	-28.17787543824361	0.22456773634220
N	33.09922756073830	-25.45812869091079	4.86220232459825
N	34.48111451606663	-25.59297493577975	7.34778045041468
N	34.80119528926210	-27.55029739377294	3.80723716307581
C	32.96182110510774	-26.44790901977218	2.62711506646748
C	32.72411892155456	-23.98707640923146	6.78142428254144
C	36.24348691088174	-26.78243117709732	8.56598914104311
C	36.76101391709106	-28.93010982322101	4.27242566849235
C	30.54321549560238	-22.71031301220315	4.97913399429425
C	33.20348967153312	-22.92356803852408	9.65986247425004
C	38.67511617444597	-28.67085366341157	8.92357061082581
C	36.46530934056447	-29.81026848318124	1.31601012782418
C	32.54942193322072	-25.55891299674823	3.61681602211164
C	33.66862561955364	-24.53691125378743	7.64712921656904
C	36.69242603367727	-27.62906442987708	7.55544539237975
C	35.75892804211136	-28.44377358645163	3.43988644577857
C	31.49634480940427	-24.56576414798745	3.44289246005612
C	33.91552108373075	-24.07083017408499	9.00528035514678
C	37.84711189152712	-28.51265975722426	7.68187703251486
C	35.58691730597892	-28.83747450353212	2.04505721482402
C	31.44068755263803	-23.85505998517495	4.61164965812351
C	34.89628950710027	-24.87867094319737	9.51510529973908
C	38.01060019712620	-29.10490926192014	6.45904349730517
C	34.49658618406722	-28.15367354124634	1.58825909415499
C	32.45466257333067	-24.42885455922579	5.48685777004975
C	35.24204300576861	-25.82070904315515	8.45823674814524
C	36.94575560540496	-28.58456078833566	5.60857244451120
C	34.02659648654286	-27.34141710617491	2.70779319529968
N	36.16523809891002	-27.70954715894227	6.30082137908210
Fe	34.57377610330181	-26.65174581204699	5.60393344040137
C	33.81420258985975	-31.38287848181413	7.34812425688830
C	35.27370617847188	-31.78190570912452	7.18123392848260
C	32.11000879828627	-27.58257298270723	6.99781801266975
C	33.35988052257912	-27.89314131279737	6.21176605957273
C	33.53448829703083	-29.36143203123155	6.08978336944794
O	33.58316003875444	-30.02117429289125	5.07458184639623
O	33.63959562091043	-29.95860355538734	7.33482089553106
H	29.83338675002524	-22.47954037346436	4.17668394384790
H	31.11165946999561	-21.79215706510977	5.18567885111833
H	29.95518579122410	-22.92735540288435	5.88209209801638

H	31.29920191586195	-24.10512937149803	1.33640200348203
H	30.15759893057297	-25.31791983280431	1.91775763190822
H	29.91633592929033	-23.61359971565596	2.32178753450469
H	33.86845399628908	-27.18201556470728	-0.24098471780618
H	34.41346999534328	-28.85017486580324	-0.45149915050477
H	32.82890883453623	-28.51857130745269	0.25869857751200
H	36.17841840373654	-29.90105394981303	0.26227992816204
H	37.52063850919703	-29.50492400522572	1.34214978790927
H	36.41333359487842	-30.81573418763546	1.75715873625918
H	33.56626835799563	-22.75371568246378	10.67981784104116
H	32.11965232873641	-23.09686537044657	9.72296125930448
H	33.34125252249456	-21.98598624886451	9.10282179682965
H	36.62046990829002	-24.66134249148561	10.80402614890269
H	35.40791712633279	-25.78819784381263	11.41165519083684
H	39.48559442679374	-29.39340805056469	8.77630236157070
H	39.13506038118297	-27.72119483345623	9.23192872767573
H	38.07486591331966	-29.02277459363365	9.77453983868411
H	38.61761951800550	-31.03359076948716	5.68538360373573
H	39.63921148248022	-29.69202417738324	5.16532769926507
H	39.76699499465445	-30.31054547349483	6.81707631754323
H	35.11301330984675	-24.04699459970740	11.49589867846358
H	35.89792197680992	-31.29281076906845	7.93294254962927
H	35.38614934834945	-32.86819154064577	7.28286359216755
H	35.63659719792397	-31.48468285449156	6.19679390201210
H	33.20202746983839	-31.82751819655018	6.55963496179663
H	33.42778649010990	-31.70020920577826	8.32102629802677
H	31.89240924048759	-26.51848833272135	7.03355411001374
H	31.22966362493215	-28.10228802223592	6.58593449409030
H	32.22561862948672	-27.95043867207648	8.02713131486015
H	32.43270292887954	-26.40245525575995	1.67927635475617
H	36.76490910466599	-26.83875859113420	9.51751681901315
H	37.46016543417463	-29.64248546479937	3.84385785260604
H	32.14020851228144	-23.14946818090732	7.15219431489800
O	35.83263667411852	-25.36815416342263	4.96772304308224
H	35.50116965210457	-24.48806564359840	5.19922792665361

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B3LYP Scan/Hydroxide IPC Model/RKS/130 degrees Constrained Optimization

C	30.68693498904031	-24.34839350101313	2.18678768925759
C	35.51539174067106	-24.96096655080246	10.86692904362764
C	39.08991110078031	-30.06305254706393	5.89943324661960
C	33.87050092581588	-28.11693298574977	0.16069259179070
N	33.10192439451752	-25.46549916646326	4.83705400344974
N	34.47852951897575	-25.64185474135521	7.32390938166185
N	34.79593802994528	-27.54572474671801	3.75340914337852
C	32.95517003967796	-26.42720046672697	2.59019747800789
C	32.72954739371286	-24.02083310911376	6.77764455276622
C	36.24027083464131	-26.85047524540946	8.52420953662792
C	36.77134833940548	-28.91221925015912	4.19009977784890
C	30.56652634156773	-22.69971038120579	4.98817435997079
C	33.18947408245958	-23.01861687400845	9.68073615560138
C	38.69895810520546	-28.71300338860301	8.83739890920438
C	36.47437940023003	-29.75018369838026	1.22277753549407
C	32.54978465472306	-25.54753221643709	3.59101237129620
C	33.86529653202537	-24.59175836787785	7.63911991831761
C	36.69636409527619	-27.67364957875186	7.49700326220554
C	35.76090171349463	-28.42464452230603	3.36993225213793
C	31.50392374908564	-24.54493995917553	3.42982106788358
C	33.90484802516350	-24.15297513900586	9.00765538181656
C	37.86380289037375	-28.54276699013811	7.60228285062707
C	35.58934170007505	-28.79680205990889	1.96926039632474
C	31.45448215590752	-23.84744646171944	4.60692410597347
C	34.88222843004019	-24.97140347225463	9.50687595321210
C	38.02992255121051	-29.11031036844618	6.36815006922713
C	34.49303649197084	-28.11395016632091	1.52493146050551
C	32.46388969005195	-24.43925106023601	5.47478359539097
C	35.23451549110488	-25.89161071157951	8.43307090170276
C	36.95461009332204	-28.58949572954956	5.53144010175234

C	34.01952561202150	-27.32263864340192	2.65799105488620
N	36.16474737450132	-27.73864010495142	6.24305360146026
Fe	34.57157658877485	-26.67449694089013	5.56536311388965
C	33.75085213472363	-31.33264940349477	7.54633731854059
C	35.23569207049015	-31.60496375392495	7.74189067774042
C	32.06624795064774	-27.60208196818783	6.88413259155729
C	33.35745456185250	-27.92105651436068	6.17155284364390
C	33.60331503357711	-29.38371922883054	6.15357187877257
O	33.88781699938707	-30.08386212720644	5.20660657421194
O	33.48045658608856	-29.93053869555946	7.42566346823306
H	29.85611729925683	-22.45605621793517	4.19011512925741
H	31.14253324870046	-21.78788471707222	5.20172443983556
H	29.97970154078647	-22.92115088212385	5.89078499310146
H	31.30843249725891	-24.04660414956891	1.33152611393944
H	30.16664062778543	-25.26982982742273	1.89031149866703
H	29.92483197162352	-23.57321402234241	2.32467221336709
H	33.86689876752708	-27.11406766040324	-0.28971497158320
H	34.41020343948832	-28.77934517416018	-0.52526614505084
H	32.82534243425039	-28.45661429141310	0.18843043464200
H	36.18278416942005	-29.83042794851465	0.16946431289526
H	37.52635896957581	-29.43336133901833	1.24734152967312
H	36.43594602457760	-30.76154393232378	1.65141335338857
H	33.54364540438505	-22.87146291305421	10.70721405297967
H	32.10487172557296	-23.19109307909105	9.73074323882911
H	33.33379645780168	-22.06941850911832	9.14542217017503
H	36.59897722983305	-24.78584957047126	10.81028056638798
H	35.37746748646462	-25.91806103493274	11.38961444248031
H	39.51912875524128	-29.42073945349787	8.67301194659099
H	39.14631350601327	-27.76290715759187	9.16232783958708
H	38.10776714940464	-29.09015208171699	9.68395612066334
H	38.66063169395669	-31.01119787552055	5.54657568387254
H	39.66732425496623	-29.64503487457725	5.06295015980761
H	39.79978839617023	-30.30434568338410	6.69873715854344
H	35.09010985426499	-24.17728796407326	11.50388625869750
H	35.61806160673879	-31.05841235342869	8.60766882749394
H	35.41214795522104	-32.67614340800640	7.89785899687863
H	35.79806073745340	-31.28325448860086	6.86459832898321
H	33.37894388565731	-31.84919307459454	6.65843028679207
H	33.17235818111578	-31.65636212248222	8.41672137083191
H	31.81328054144645	-26.54656303199295	6.83637193575333
H	31.22035632590270	-28.17901555822357	6.47698244142603
H	32.14856816718515	-27.89352854056936	7.94005261090407
H	32.42512642011326	-26.36787094169490	1.64367722951045
H	36.76208103799163	-26.92105985787063	9.47452342709713
H	37.47541949463938	-29.61129651708898	3.74815647611131
H	32.14755509293424	-23.18726791099962	7.16023011366958
O	35.83503732737264	-25.38728843475066	4.94993713148904
H	35.47214588736644	-24.50716289008049	5.12817384869522

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B3LYP Scan/Hydroxide IPC Model/RKS/140 degrees Constrained Optimization

C	30.66921474687937	-24.37472786538314	2.20036041950877
C	35.51107837887062	-25.00714554379217	10.87026196082471
C	39.10865234463495	-30.06315806055436	5.86863706264476
C	33.88724775464452	-28.09711291627407	0.14140568089317
N	33.11460581725769	-25.47144802563964	4.83074272773768
N	34.49678574371048	-25.65203159433583	7.31434283364703
N	34.81395458483660	-27.53886062972121	3.73598963879653
C	32.95853345144467	-26.43311956784026	2.58454878127150
C	32.74572356258561	-24.03092591124694	6.77523716402037
C	36.24767014667119	-26.87702462457185	8.51420990513667
C	36.80546221457616	-28.88545948863437	4.15909923808071
C	30.561352503323200	-22.72317428475337	5.00055238881310
C	33.19563768152528	-23.05023448084360	9.68753770302917
C	38.69610177930456	-28.75608341756609	8.82360391313412
C	36.51760431382359	-29.69989986604237	1.18517341512702
C	32.55317860303718	-25.55796516103017	3.58922862547818
C	33.68231484331250	-24.60420853375343	7.63418277147401

C	36.70833581021399	-27.69057645736889	7.48126420098452
C	35.79028956503489	-28.40106635279844	3.34368678267412
C	31.49904201753648	-24.56295531990743	3.43622877159405
C	33.91537626039425	-24.17769311239575	9.00747641775130
C	37.87253965248652	-28.56467896779267	7.58394101333278
C	35.62068134465849	-28.76483403499132	1.94070964613450
C	31.45508848887895	-23.86426080241334	4.61289529548604
C	34.88827095098363	-25.00253971880942	9.50538818485937
C	38.04771851955263	-29.11417025998471	6.34286039381901
C	34.51299135749206	-28.09520092335100	1.50423481856525
C	32.47523851577845	-24.44878518572360	5.47318952522459
C	35.24579542621020	-25.91348564580374	8.42565864465316
C	36.98003581896100	-28.57951078234402	5.50510646485764
C	34.03214918039231	-27.31800136032165	2.64399520558489
N	36.18604302903930	-27.73823680430932	6.22254005993997
Fe	34.59064835992598	-26.67627814044611	5.55179482692166
C	33.64138190356713	-31.35425423137215	7.53964687972003
C	35.10069432005230	-31.60040326839029	7.89989652566756
C	32.11221860621084	-27.59138450020355	6.91514290613897
C	33.38154809242923	-27.92676086951744	6.16973221039471
C	33.63544512839358	-29.38706029737069	6.16193913184510
O	34.05427090163668	-30.07449356868564	5.25604317786030
O	33.35491950942304	-29.95821320233573	7.40183322555328
H	29.84160297139019	-22.48699372512052	4.20865059787996
H	31.13171767282993	-21.80619402708054	5.20703680188577
H	29.98477136474872	-22.94781193256630	5.90891581111827
H	31.27878399047397	-24.05990777468124	1.34115994347102
H	30.16144994450315	-25.30335653284880	1.90482423931612
H	29.89591612295804	-23.61240839370395	2.34727299665849
H	33.87379141239340	-27.09218760008705	-0.30420545258321
H	34.43132135850166	-28.75143939058759	-0.54885972784828
H	32.84521594857064	-28.44618571807591	0.16980456296480
H	36.22265505342326	-29.77939474963522	0.13275169789221
H	37.56436474729516	-29.36605640795082	1.20699784327994
H	36.49752845938018	-30.71386931635092	1.60883782839666
H	33.54434964069618	-22.91242966289736	10.71715570251429
H	32.11104889929796	-23.22458499087443	9.73046307508764
H	33.34146592283376	-22.09592214088861	9.16187578363965
H	36.59636851441243	-24.84019727147448	10.82311025642446
H	35.36160105636797	-25.96694442433335	11.38481612155093
H	39.52034533149801	-29.45774470303154	8.65370007030515
H	39.13701187286087	-27.81095375190056	9.17099896064065
H	38.09774625464831	-29.15148972778392	9.65665326326373
H	38.67843297101683	-31.00305705402444	5.49575520562113
H	39.69594694038904	-29.63359864220907	5.04491932199311
H	39.80967241939624	-30.32068685577163	6.67066774652320
H	35.08706193178943	-24.22488361815330	11.50977140521612
H	35.37421032931022	-31.04668931698851	8.80208042136223
H	35.27664663818835	-32.66803735380464	8.07898183293008
H	35.75314188348795	-31.27153388732149	7.09019646600105
H	33.38293776693362	-31.87026559733608	6.61191094820666
H	32.97633172354937	-31.69914825733464	8.33712961928234
H	31.82190749562479	-26.55164422690347	6.79228996088084
H	31.26754108863138	-28.22771363037900	6.61002346964744
H	32.25755348229797	-27.78042863874785	7.98745060885653
H	32.42301266107272	-26.37569358883912	1.64101126041211
H	36.76293032324630	-26.95889810552319	9.46719498482638
H	37.51581261557327	-29.57447503163982	3.71146876437167
H	32.16179435162126	-23.20058390532227	7.16182481939306
O	35.84831724835211	-25.38449595505842	4.93960394014424
H	35.48675951383608	-24.50625385715018	5.12973965129333

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B3LYP Scan/Hydroxide IPC Model/RKS/150 degrees Constrained Optimization

C	30.63669394474832	-24.41798194152949	2.21938831322439
C	35.52054968621360	-25.02825852957637	10.86493026507395
C	39.15780524365566	-30.01983833642878	5.82588057834259
C	33.89853129679481	-28.08440639342748	0.12670618921330

N 33.12557888215552	-25.47731404754052	4.82416614120583
N 34.51875245315549	-25.65265125011286	7.30201123614399
N 34.83777137942559	-27.52192742354769	3.71749249864011
C 32.95655918785192	-26.44485623085346	2.58150819695701
C 32.75535725715669	-24.04174882483937	6.77250198336216
C 36.27106876214611	-26.87918148611349	8.49797305169949
C 36.85720619272509	-28.83212704682175	4.12233541448187
C 30.54298387927252	-22.75754323328876	5.01470575400740
C 33.19888268938008	-23.07398514097450	9.69001229812086
C 38.72326667047145	-28.75535794482803	8.79756017752555
C 36.56984873702603	-29.63499845311061	1.14586341936424
C 32.55048065685919	-25.57382473565602	3.58940555771176
C 33.69749830563237	-24.61167756169639	7.62716160203714
C 36.73949845148952	-27.67917554919223	7.45798142803120
C 35.83003406618433	-28.36120927517417	3.31473789577561
C 31.48272670242197	-24.59259868329952	3.44637494302776
C 33.92600093901333	-24.19281470692832	9.00354822245643
C 37.90635136491162	-28.55097254267791	7.55564514261624
C 35.65902241314731	-28.72155932484892	1.91123295548430
C 31.44475060182884	-23.89037010494436	4.62133742556806
C 34.90127318569495	-25.01680794389362	9.49848974008646
C 38.09101587630603	-29.08143533867766	6.30767830482737
C 34.53368070873010	-28.07467640619718	1.48519233999982
C 32.48064702330957	-24.46086645493412	5.47173047822305
C 35.26587358308996	-25.91853694106932	8.41360069803234
C 37.02517777652807	-28.54005578218275	5.47175264964385
C 34.04503117642714	-27.31189390556414	2.63115014692145
N 36.22372679200885	-27.71333686176393	6.19663041375853
Fe 34.61506848149126	-26.66838072961460	5.53609733493803
C 33.51378154325096	-31.39727981392455	7.46676023212998
C 34.85919476892493	-31.61595187731887	8.14752574346007
C 32.16118553202968	-27.59082927581175	6.92550598067480
C 33.42042575016892	-27.93086097608735	6.16396367714148
C 33.68604512274420	-29.38918244073908	6.15444069926791
O 34.24740794705982	-30.04926219297162	5.30662798931475
O 33.22284953238682	-30.00457407354159	7.32110595806495
H 29.80361758806489	-22.54123736631804	4.23530429108273
H 31.10415656253100	-21.82996009623842	5.19802062781346
H 29.98901308293480	-22.97916234881069	5.93763107657129
H 31.22527164254410	-24.06146547686683	1.36164375163030
H 30.16775187695426	-25.36240056571412	1.91083814072374
H 29.83219403905137	-23.69269482760979	2.38534061991426
H 33.86023635189012	-27.07806879161905	-0.31413886033303
H 34.45205032450628	-28.72365018912863	-0.57016836367965
H 32.86450113033048	-28.45613416502655	0.16045493692007
H 36.26595076359396	-29.72111471978780	0.09652341550270
H 37.60872921388301	-29.27683170781674	1.15724641632553
H 36.57772446221911	-30.64915056054269	1.56942737311635
H 33.54390637851866	-22.94245299680050	10.72168677445915
H 32.11508999628031	-23.25402041283517	9.72839251805735
H 33.34163231374474	-22.11493964842298	9.17221070486593
H 36.60478005774232	-24.85334907411268	10.82207601605954
H 35.37638856727227	-25.99320766193910	11.37127211057866
H 39.54873210908772	-29.45491829293004	8.62472342977586
H 39.16198601381639	-27.81380121869025	9.15732706117894
H 38.11990760720577	-29.15959124466159	9.62262035599112
H 38.73159507656074	-30.95390697362727	5.43462371311982
H 39.74998492167696	-29.57541741264744	5.01355735311687
H 39.85366550725496	-30.28880962048440	6.62864711411848
H 35.08945579486452	-24.25420021246325	11.50964497788177
H 34.88812204831478	-31.10513292128090	9.11409985962954
H 35.04007684356260	-32.68481297225751	8.31344914061255
H 35.66776727937108	-31.22079704113242	7.52976543192345
H 33.49819806252698	-31.87473061386059	6.48473239197480
H 32.69753800137733	-31.79974276960795	8.07486931153546
H 31.81426650860729	-26.58221705854181	6.71686654219856
H 31.34100351165009	-28.29567296317509	6.73194265244738
H 32.36221050164256	-27.65484424303818	8.00451606888062

H	32.41172189653131	-26.39521019209598	1.64294582683961
H	36.78271050712149	-26.96847260303780	9.45220465957598
H	37.57690043328959	-29.50680833236384	3.66789563089403
H	32.16599502386543	-23.21745962087624	7.16367698033758
O	35.85912744531989	-25.36484853658653	4.92471395938215
H	35.49134514347239	-24.49003830834795	5.11900225442081

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B3LYP Scan/Hydroxide IPC Model/RKS/160 degrees Constrained Optimization

C	30.60311976349610	-24.49191555291131	2.25905147708698
C	35.57607181925992	-24.95647989976807	10.86249708681564
C	39.24939539453533	-29.91752468337840	5.82500214744315
C	33.88736191138096	-28.13984607463777	0.17204153483559
N	33.12704724800761	-25.49787432691094	4.85082651521656
N	34.54709378248403	-25.63100820459536	7.31674848257635
N	34.86169851070081	-27.52410916102066	3.74435348575083
C	32.94302061240673	-26.49652910445246	2.62334073287305
C	32.77168370862417	-24.03476244100481	6.78128532003415
C	36.31946970379291	-26.82956971494924	8.50920133584373
C	36.92349150264342	-28.77102156000760	4.13108554096589
C	30.53449681266839	-22.78760317228125	5.02946815613712
C	33.23735812677305	-23.02641584199963	9.68184748030000
C	38.79714819299907	-28.67117871232610	8.80217920208339
C	36.61955911984196	-29.60105322523911	1.16168726708345
C	32.53883695599981	-25.61654638598604	3.62438151141929
C	33.72403842399294	-24.58918954832533	7.63512628461867
C	36.79344513972470	-27.62539039437871	7.46854005558127
C	35.87284410645037	-28.33633578499089	3.33329185222151
C	31.46474342794284	-24.64252697549015	3.47824274302100
C	33.96210149650635	-24.15211745070654	9.00411961413982
C	37.97683182584105	-28.47578609698461	7.56116845958501
C	35.69238922145395	-28.71096701871608	1.93490512883314
C	31.43749163779216	-23.92154104644391	4.64220512379547
C	34.94430703105338	-24.96627404418086	9.50175564843556
C	38.16952722533367	-28.99707648176484	6.31122355039302
C	34.54182715009387	-28.10097934559726	1.52091506102069
C	32.48522243909275	-24.47423197701884	5.48963926075166
C	35.30462973718272	-25.87930281160342	8.42507586959474
C	37.09063209447757	-28.47543397853786	5.47949151553919
C	34.04844639255732	-27.34259680253177	2.66770088585525
N	36.27471826129994	-27.66740032606684	6.20909932108885
Fe	34.64455799102075	-26.66231546760436	5.55956143352483
C	33.27837232978684	-31.49018480066802	7.27095252247310
C	34.53420607211131	-31.81265214344550	8.07252865420716
C	32.19404373757429	-27.60435522908655	6.93448196747261
C	33.46816790748434	-27.94319128598815	6.19896823102896
C	33.72779330919991	-29.40177720502650	6.17117764634679
O	34.44322610859331	-30.02782114734532	5.41641851912616
O	33.04514360378386	-30.08306008478832	7.18749969265309
H	29.80570073894926	-22.56457149980286	4.24205000185682
H	31.09679872169803	-21.86335663041488	5.22488723812201
H	29.96759042441129	-23.01170187151007	5.94412261787231
H	31.19053654802531	-24.20518200032470	1.37507934201805
H	30.08704756601385	-25.42857573030552	2.00594077163660
H	29.83434551089116	-23.72427153391290	2.40190697907519
H	33.80567262037180	-27.13745065456257	-0.27166767054328
H	34.45376779889610	-28.76103739909440	-0.53081573049329
H	32.86815330923304	-28.54893211598175	0.22224029852448
H	36.29609829855507	-29.71333746506066	0.12071037298631
H	37.64449931133883	-29.20471680886827	1.14535228033900
H	36.67440860436071	-30.60799382775420	1.59865523463701
H	33.59406142853405	-22.87714609712310	10.70712169618785
H	32.15492690481400	-23.21075351880872	9.73593798663141
H	33.36940305328167	-22.07494235445755	9.14748549855929
H	36.65759625874944	-24.76827731460302	10.80818918205695
H	35.44874952035801	-25.91825506573967	11.37921411830176
H	39.63009344134420	-29.36167960670645	8.62872773690659
H	39.22588413315406	-27.72506697387020	9.16230003335071

H	38.19844466514358	-29.08196613329318	9.62742935421972
H	38.83604214937480	-30.85960873218021	5.43908652321671
H	39.82842496893188	-29.46523796849664	5.00753811150576
H	39.95520522169642	-30.17228971736006	6.62374375289891
H	35.14085425573927	-24.18186104948530	11.50376357662728
H	34.48010353006187	-31.36673424170417	9.07003987407889
H	34.65260493822149	-32.89722042750441	8.18405556484511
H	35.41702955080049	-31.41865301539264	7.56670640511618
H	33.35328110850222	-31.90727286948647	6.26375016322480
H	32.38796937985882	-31.89693654555295	7.76054368143408
H	31.92751255651298	-26.55637258872701	6.83680602525803
H	31.34469565077880	-28.21448236063993	6.59565198655574
H	32.30724748429135	-27.82679979826967	8.00476374653317
H	32.38544157516270	-26.46714760268328	1.69138577574689
H	36.83777185578776	-26.90849910261034	9.46075716777722
H	37.65886512461720	-29.42529645736396	3.67188879359539
H	32.18253514877654	-23.20762488758201	7.16672904286539
O	35.85552303876116	-25.34276096282362	4.92398603523913
H	35.47446292103648	-24.47162510418315	5.10914945546307

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B3LYP Scan/Hydroxide IPC Model/RKS/170 degrees Constrained Optimization

C	30.57165453108319	-24.56982851331013	2.29942579472808
C	35.62710240524367	-24.87574325339298	10.86150988520056
C	39.32931357163884	-29.82583080967520	5.84173246228439
C	33.86553017107328	-28.22397140681318	0.23368610859431
N	33.13095229642325	-25.51469991184134	4.87888852676486
N	34.57476950403069	-25.60297397054293	7.33306459973087
N	34.88439649794636	-27.52575787016974	3.77809634478467
C	32.93158549777183	-26.55017503725959	2.66974312401203
C	32.78747022084621	-24.02271985734846	6.78924650388427
C	36.36395781558669	-26.77426425817257	8.52618949614505
C	36.97745450929780	-28.72368640930150	4.15353021987625
C	30.52450968142668	-22.81750310353285	5.04037298178122
C	33.27551804893634	-22.96789586676870	9.67038135398248
C	38.86364850247474	-28.58401902600550	8.81834690711348
C	36.64639982553201	-29.60594362813025	1.20121061491371
C	32.52986253579167	-25.65849541229547	3.66149965105940
C	33.75050670156484	-24.55915439733824	7.64279601832508
C	36.84257763711808	-27.56945285610265	7.48728902817188
C	35.90724740642205	-28.32200317940439	3.36402279870008
C	31.44735869518676	-24.69448446578005	3.51151620994195
C	33.99724774501346	-24.10210036125498	9.00364937262444
C	38.04001397110302	-28.40034083314228	7.57778860147767
C	35.71346899406574	-28.72195400482556	1.97457330949323
C	31.42906347603734	-23.95351399409224	4.66309671377061
C	34.98491242525252	-24.90693398768280	9.50589930698829
C	38.23814221139989	-28.91912806035610	6.32811426716555
C	34.54271798880758	-28.14462501754705	1.56957015091861
C	32.48943985704310	-24.48537476441802	5.50816390782432
C	35.34096555320092	-25.83308829154250	8.43920553052558
C	37.14726995948964	-28.41817324855903	5.49912695267424
C	34.05135793584132	-27.37765731838329	2.71134410450456
N	36.31993588972394	-27.62327495112279	6.23034371411202
Fe	34.67049472511992	-26.65003253358688	5.58463777871307
C	33.08970503661794	-31.55494027441850	6.98700862072642
C	34.22539371556610	-31.99313215223605	7.90517338732717
C	32.25638516931870	-27.60512954027700	7.00519787356381
C	33.51223339952082	-27.94188160304125	6.23833414070512
C	33.74784638893880	-29.40184758380540	6.15252631884019
O	34.56296545563332	-29.99596562383714	5.47559165682100
O	32.90597619052197	-30.13862488036105	6.99807966108054
H	29.78983382998850	-22.60795087436552	4.25470911965537
H	31.08499010990029	-21.88879847774404	5.21905794588922
H	29.96428180191597	-23.03046735268073	5.96179522133739
H	31.14943498420681	-24.30459896471611	1.40255963776822
H	30.05084859120449	-25.51089028386885	2.07356692200952
H	29.80607150101870	-23.79745903003704	2.43364785045634

H	33.74355371511214	-27.23138688462590	-0.22247336201456
H	34.43879801445341	-28.83711723421480	-0.47070435768423
H	32.86102236881555	-28.66452438224163	0.30860162883407
H	36.30769636507272	-29.74390017357054	0.16819018034886
H	37.66222201778216	-29.18844385432532	1.16024868598768
H	36.73020092695200	-30.60340078080488	1.65497116547056
H	33.64157576137315	-22.80157622888355	10.68972599517831
H	32.19412966068943	-23.15405808788741	9.73755347977586
H	33.40011518861037	-22.02469529278908	9.11980006870102
H	36.70679999116331	-24.68043911506577	10.79662790587044
H	35.51073904238503	-25.83201902657617	11.39080944339702
H	39.70454091368141	-29.26493590387443	8.64533823241840
H	39.28131022873337	-27.63254713064450	9.17745277927991
H	38.26997619093690	-29.00082596136638	9.64428579824527
H	38.92780337237537	-30.77607525375503	5.46326861893990
H	39.89788049371762	-29.36988545360324	5.01897430886935
H	40.04252926048704	-30.06577408662526	6.63853629588696
H	35.19106736698502	-24.09653644371990	11.49662862937061
H	34.05869213026923	-31.63522333583915	8.92551467058116
H	34.29957423090583	-33.08703506520511	7.93106641340669
H	35.17419484920362	-31.59038502709543	7.54792941401978
H	33.28057054520561	-31.88882009227860	5.96407085075338
H	32.13374060252336	-31.96735275342773	7.32443873809184
H	32.02834393131479	-26.54418634695127	6.97762599368328
H	31.38541657800655	-28.15909741043820	6.62817202417313
H	32.35830120678920	-27.90446320397400	8.05819181153780
H	32.36119703011030	-26.54368620268615	1.74511619338990
H	36.88809686751455	-26.84100950056185	9.47548693569794
H	37.72251723358507	-29.36555115724609	3.69240038992258
H	32.19790243219633	-23.19237930207506	7.16710099407357
O	35.85706517874895	-25.31747735667920	4.93298067330691
H	35.48452249545481	-24.45028825288023	5.15105804551946

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B3LYP Scan/Hydroxide IPC Model/RKS/180 degrees Constrained Optimization

C	30.53400825253123	-24.67795824489039	2.36194280489272
C	35.70880760754068	-24.77435590344965	10.85843374578392
C	39.44342775110225	-29.70698161722274	5.85177394027455
C	33.84483308748860	-28.32874181625829	0.31545601593178
N	33.14103109887470	-25.54277087982590	4.92115780420867
N	34.62112438908491	-25.57035995954406	7.35584176425549
N	34.91525219185475	-27.53924418951436	3.82540850929319
C	32.92556774095362	-26.62019187025500	2.73367653396860
C	32.80534534735431	-24.02299634532471	6.81034164750998
C	36.44507609921559	-26.69406751334052	8.54092204034448
C	37.04017125033692	-28.68537699229283	4.18520925777086
C	30.50312792758251	-22.87661600929563	5.07120207520768
C	33.31739118705939	-22.91550946424985	9.66860337003350
C	38.98548213971550	-28.44650547039597	8.82077650777350
C	36.67169973509424	-29.63334728692963	1.25581170085874
C	32.52503477250249	-25.71666403786534	3.71527999556316
C	33.78707130397047	-24.53224925804517	7.65961957646476
C	36.92602985526022	-27.49117090632229	7.50479109448165
C	35.94654372894032	-28.32303853836362	3.40794875084942
C	31.42778810928451	-24.76975276709465	3.56381528399737
C	34.04489217461382	-24.05085715685229	9.01015771333710
C	38.14372148654076	-28.29299572718423	7.58831984876839
C	35.73579622228849	-28.75307719367110	2.03000367040490
C	31.41627321456647	-24.00833871863271	4.70216011930865
C	35.04940463572553	-24.83485614278835	9.51205707512465
C	38.33808770820011	-28.81969271895293	6.34187979765432
C	34.54617975767794	-28.20701699382811	1.63572898936524
C	32.49504718489605	-24.51147610556088	5.54162235933126
C	35.40470043908123	-25.77220713515832	8.45504887222275
C	37.22405425415190	-28.35477034548290	5.52258658571143
C	34.06036064691430	-27.42749122255225	2.77111858794895
N	36.38809371919363	-27.57089338408549	6.25614167068888
Fe	34.71087518417514	-26.6396600759850	5.62085662588264

C	32.86070771077444	-31.57400405034059	6.61640877527700
C	33.74896831246577	-32.18143914912378	7.69648691580127
C	32.32005358733111	-27.60961393245514	7.06516492704413
C	33.57520414577247	-27.94230697034683	6.29475682320280
C	33.77702338580965	-29.40214481466538	6.14484205890166
O	34.68250207630419	-29.98586890530115	5.58269774099075
O	32.75604002791598	-30.15620577642279	6.74356253812941
H	29.75898459190970	-22.68642334220737	4.28951529656748
H	31.05548127192322	-21.93964713361646	5.23082960802766
H	29.95368216008436	-23.08156957801472	6.00092985287869
H	31.09718855654481	-24.42848588539793	1.45142299189139
H	30.01694441209318	-25.62737557888066	2.16396170956669
H	29.76476169017846	-23.90820164591608	2.49006309289785
H	33.68207825979870	-27.34790428022524	-0.15304090231486
H	34.42277774431803	-28.93477595464054	-0.39130264860563
H	32.85651463799366	-28.79936999253433	0.41798571841819
H	36.31731758979185	-29.79620960472351	0.23168085938763
H	37.67845085502042	-29.19763201605851	1.18905360765350
H	36.78279625848672	-30.62076360826510	1.72536987613039
H	33.69390820630684	-22.72958843664291	10.68073400216286
H	32.23923674612780	-23.11353207374687	9.75185317360505
H	33.42396406900327	-21.97933201974215	9.10246005492860
H	36.78362826417002	-24.55923567191871	10.77692674706320
H	35.61781031179633	-25.72621218097947	11.40045762525674
H	39.83594537961502	-29.11489866291292	8.64570107317945
H	39.39063583132850	-27.48368844251795	9.16371190123570
H	38.40890959466358	-28.86353825665901	9.65864295521870
H	39.05860441037103	-30.66956696808105	5.48735237610873
H	39.99296347263443	-29.24722820858365	5.01819853813962
H	40.17056976023073	-29.92349016043841	6.64274205898985
H	35.26603489178888	-23.99605264978770	11.48994328156558
H	33.38777967411653	-31.90877494569983	8.69267549234669
H	33.75681796441810	-33.27553128089675	7.62093695989450
H	34.77291075263416	-31.82075654073095	7.58731678117129
H	33.24662163116751	-31.82344674528597	5.62487440433237
H	31.83431513828479	-31.94389068163857	6.70347862587131
H	32.16183568942501	-26.53997062019632	7.15667866975916
H	31.43337135531871	-28.05009008886391	6.58850311842013
H	32.35092255713636	-28.03985604036832	8.07641111077078
H	32.34045305783258	-26.64025383918423	1.81848593741129
H	36.98263684008475	-26.73929875156571	9.48396456982955
H	37.79235607737132	-29.31714428502646	3.72167524518764
H	32.21002429177781	-23.19413526542757	7.18243140636196
O	35.86141503080675	-25.29143495669008	4.94015867588744
H	35.49146067629972	-24.42945562744982	5.18190138024235

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B3LYP Scan/Hydroxide IPC Model/RKS/190 degrees Constrained Optimization

C	30.50945503105088	-24.75905850000260	2.41149616441496
C	35.78510199128658	-24.67301371830592	10.84845991366316
C	39.51073431180534	-29.64010657300344	5.87147567677467
C	33.82258162103071	-28.41748758134270	0.38899099954864
N	33.13790152179514	-25.57454346280926	4.96500551743226
N	34.65450628268093	-25.54298418328561	7.37732648200955
N	34.92947528100175	-27.56054370358696	3.87216997141363
C	32.91612870997552	-26.67990267148651	2.79161882210621
C	32.80858089677593	-24.03010732778112	6.83447131106460
C	36.51220663738976	-26.62073017424294	8.55224129964000
C	37.07360445647706	-28.67420053685585	4.22163041962150
C	30.48274454469815	-22.92509125383658	5.09831852000396
C	33.34993280100547	-22.866691732836721	9.66555150248700
C	39.07379881493337	-28.34281141767462	8.82707142673641
C	36.67350340066917	-29.67914164239015	1.31347003563885
C	32.51503960938439	-25.76842921395501	3.76576639922274
C	33.80993676016158	-24.51169575505791	7.67705739541540
C	36.99010323142516	-27.42607173477339	7.52140944433788
C	35.96361906718400	-28.34050226156835	3.45392651837014
C	31.40927473245294	-24.83217480248326	3.61024192620577

C	34.08158129329301	-24.00441436212791	9.01541544312809
C	38.21780842795858	-28.21305032829417	7.60169989289209
C	35.73934461764214	-28.79543886518279	2.08608017913275
C	31.39938277129011	-24.05717555452594	4.73939347603239
C	35.10491945316152	-24.76578413520366	9.51429265245578
C	38.40300725990327	-28.75537669784156	6.36090670980763
C	34.53950207794491	-28.26694997282073	1.69805720466264
C	32.48808209312880	-24.54123749349433	5.57734352585206
C	35.45743752277760	-25.71525731561871	8.46731566867937
C	37.27347329593506	-28.31516880647690	5.54901938143800
C	34.05991533507241	-27.47449580811972	2.82685549160960
N	36.43789803748205	-27.52965125715568	6.28104058943644
Fe	34.73552589890611	-26.63542804288479	5.65696916288074
C	32.73659877150277	-31.55133353139534	6.28586019989256
C	33.40424600692062	-32.28203462036105	7.44577820597680
C	32.37713287160571	-27.62725457922287	7.14004741836488
C	33.62750242022691	-27.94731696274474	6.35600190538840
C	33.80669077197990	-29.40314497885205	6.15170638300615
O	34.77540677836429	-29.99237227179498	5.71567279386071
O	32.66841438085555	-30.14277180245599	6.50642673976806
H	29.73426421964614	-22.74809780047373	4.31764682077085
H	31.03195839197729	-21.98389477803996	5.24314859236436
H	29.93838484599421	-23.12013604339322	6.03315969520152
H	31.06779455620917	-24.51875584120979	1.49555035164775
H	29.99501509669858	-25.71268118398428	2.22730245829053
H	29.73799967767389	-23.99051594641772	2.53343414767565
H	33.63220831181214	-27.44518938109416	-0.08665821247389
H	34.40365004802963	-29.01809390542982	-0.31986860611996
H	32.84616655209223	-28.90819101081089	0.50994042102172
H	36.31010368694351	-29.85654970191634	0.29489895907836
H	37.67668462574513	-29.23796462617369	1.23147117033342
H	36.79578471363615	-30.66025827115614	1.79341906467084
H	33.73743620239551	-22.66130693081946	10.66969257744993
H	32.27512853167996	-23.07492515199893	9.76571039321765
H	33.43932347936854	-21.93866220510671	9.08355865620213
H	36.85379659703952	-24.43711373906818	10.74626001258466
H	35.72260370109482	-25.61899598258056	11.40456122164333
H	39.92698002789571	-29.00776553025306	8.65220102014688
H	39.47566789297905	-27.37259545350427	9.15262984300795
H	38.50893698702254	-28.75236302868399	9.67650314024241
H	39.12992255382935	-30.61016696878614	5.52303277901085
H	40.04932635888066	-29.18708202776197	5.02708994198370
H	40.24667721124581	-29.84120453630799	6.65839140594956
H	35.33655644114634	-23.89539393459355	11.47669072914135
H	32.89160160553459	-32.06359879070764	8.38736200099412
H	33.38040607963092	-33.36653267561017	7.28454703672053
H	34.44583114956481	-31.97003628105628	7.53578777433766
H	33.27464445490239	-31.74891203337316	5.35531045069628
H	31.69631207994910	-31.87170027594771	6.17245078055738
H	32.28837284035325	-26.56873128421817	7.36352439016640
H	31.48332972984854	-27.93309386935949	6.57805626969092
H	32.33328677656517	-28.18752911493236	8.08445513053837
H	32.32224944826601	-26.71760892518375	1.88264634391966
H	37.06288418317314	-26.64463560579836	9.48847352101689
H	37.82655378039905	-29.30551904683501	3.75871639234174
H	32.20832336562297	-23.20246002319157	7.20136567854842
O	35.85132919104456	-25.27385641820971	4.94468743158276
H	35.48531396797404	-24.41829398962876	5.21356678747483

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B3LYP Scan/Hydroxide IPC Model/RKS/200 degrees Constrained Optimization

C	30.47441796934327	-24.86750103713635	2.48519688895270
C	35.89861157877975	-24.52525398669288	10.82433832760947
C	39.57825161657987	-29.58329699537994	5.91037879927729
C	33.79967492869292	-28.52502949799118	0.48525334755143
N	33.13701432996816	-25.61385154499260	5.02468088002860
N	34.69014793144954	-25.51664139517550	7.41193072875548
N	34.94785079650364	-27.58964818090272	3.93493451997952

C	32.91025072650893	-26.74983044753773	2.86685755714726
C	32.80594410293109	-24.04854134904952	6.87554325379758
C	36.59675977818148	-26.52786001908877	8.56765586129076
C	37.10360137050111	-28.68195263445754	4.27953174350670
C	30.44532490571715	-23.00113911495870	5.14893317010150
C	33.39352409130998	-22.80358140440433	9.66201855245193
C	39.18142476270783	-28.21467492622617	8.83824980321096
C	36.66947837918104	-29.75210583162779	1.39744303882241
C	32.50639062472951	-25.83152599289492	3.83363931736423
C	33.83238297600710	-24.49437323675235	7.70735249319580
C	37.06507359468030	-27.35202072057260	7.54784744725036
C	35.98108656069461	-28.37204683171178	3.51920481367116
C	31.38513753053641	-24.91393968932507	3.67712464389113
C	34.12767853964568	-23.94689640794904	9.02481898853897
C	38.30238373549454	-28.12404904819755	7.62562143305326
C	35.74128918365846	-28.85689028263157	2.16414009940230
C	31.37341230985397	-24.12611781970440	4.79730667797895
C	35.17999508908042	-24.67343540754833	9.51543847094488
C	38.47052146441477	-28.69649004771349	6.39620806428816
C	34.53351498913543	-28.34252354367537	1.78092665110090
C	32.47703815993088	-24.58373814778037	5.63084625337235
C	35.52387104443965	-25.64372759856965	8.48472453062733
C	37.32225047795563	-28.28755153560622	5.59383977278749
C	34.06345676283094	-27.53065513975036	2.89964802746746
N	36.49146811197387	-27.49212623532913	6.32076120820209
Fe	34.76333887294604	-26.63638282123788	5.70882182262867
C	32.63881195631313	-31.47366349766531	5.87228500180293
C	32.98670871331056	-32.35736870474146	7.06484395560389
C	32.43024002759749	-27.65867778246558	7.21523694622132
C	33.68134747031289	-27.95859955647155	6.42344608586994
C	33.83316077724334	-29.40574120744381	6.14687716947404
O	34.83661411707591	-30.01836381146683	5.84505524981927
O	32.61198038648354	-30.08982021169395	6.22366994227476
H	29.68889435610122	-22.84346070623620	4.37175285834372
H	30.98413334072002	-22.05155040006599	5.27715804142744
H	29.91041164162476	-23.19028481558820	6.09042277643242
H	31.02315512243895	-24.63825052493251	1.56071514245219
H	29.96552350873661	-25.82776665538340	2.32097244466024
H	29.69838309348305	-24.10265494288952	2.60115529563423
H	33.59188375425659	-27.56377761391391	-0.00521219217405
H	34.37705967354233	-29.13249453219638	-0.22078142261042
H	32.83050848192595	-29.02378875424702	0.62928681031880
H	36.29485977845438	-29.94951282571158	0.38661562094619
H	37.67025150071512	-29.30972424209790	1.29559076493137
H	36.80052875858179	-30.72386784472501	1.89388525785638
H	33.80009824020302	-22.56676143261184	10.65166320866229
H	32.32432628243028	-23.02383244197444	9.79140352100912
H	33.45670370367728	-21.88949208370471	9.05468859546274
H	36.95431448180248	-24.25414154537374	10.68178521219678
H	35.88838430998560	-25.45888210583873	11.40415138318011
H	40.03682889279511	-28.87713384734180	8.66497206205002
H	39.58095871713069	-27.23316420263371	9.13128783583064
H	38.63566392417847	-28.60651235033692	9.70821645411139
H	39.20012416798370	-30.56328638344686	5.58783032927195
H	40.10253031650957	-29.14459967598761	5.04954418218048
H	40.32601415601614	-29.76238190901928	6.69150043979827
H	35.44257987498436	-23.74888900322605	11.44872607619487
H	32.29845245052695	-32.17450362357561	7.89558755312976
H	32.92276157170022	-33.41776691715673	6.79269366027604
H	34.00319873390626	-32.14947808195258	7.40316250466801
H	33.35591898466193	-31.62850225265452	5.06262203712346
H	31.63179665539439	-31.69486531022232	5.50568468275212
H	32.39891344049829	-26.62930264865539	7.56119497500942
H	31.54388026332057	-27.83175296657403	6.58880244092960
H	32.31333699329820	-28.32463205845993	8.08159095199323
H	32.30597734114050	-26.80855750428342	1.96590025850113
H	37.16812172633494	-26.51855938767243	9.49169197121097
H	37.85387303571601	-29.31947639485846	3.82081686618043

H	32.19730711741043	-23.22490655827518	7.23775200724157
O	35.83809437282487	-25.26346939330251	4.95417303397733
H	35.47772564328799	-24.41196596135336	5.24266416062451

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B3LYP Scan/Hydroxide IPC Model/RKS/210 degrees Constrained Optimization

C	30.43995303278752	-24.96510571117926	2.54993402016308
C	35.98943312634923	-24.40089227163154	10.79579499898277
C	39.61331921191220	-29.56817834612523	5.95345876787178
C	33.78343342410166	-28.61022073243883	0.56170747685454
N	33.13550777500793	-25.64836820904406	5.07249494875681
N	34.72168049500071	-25.49264365443329	7.43516777357157
N	34.95474683404085	-27.62611928719564	3.99020946774975
C	32.90404269821703	-26.81009599690684	2.92840264592767
C	32.80350113866987	-24.06536724612404	6.90739974626434
C	36.66541567039915	-26.45052638473066	8.57525349194161
C	37.11297536551631	-28.71283387233824	4.33645289307008
C	30.40717083873860	-23.07385189475598	5.19541948880558
C	33.42650531002165	-22.75281014813572	9.65473286355633
C	39.26177584752992	-28.11955440641630	8.84742050463108
C	36.65908421653965	-29.82502060253816	1.47191451469544
C	32.49782224127453	-25.88667687411738	3.88929160720213
C	33.85235968516481	-24.47877952956662	7.72774397567001
C	37.12150580498166	-27.29772357633761	7.56917346565790
C	35.98482678420837	-28.41518257676528	3.57900949063346
C	31.36181546285108	-24.98693078831345	3.73402711110453
C	34.16555533992529	-23.89821035251450	9.02683188246210
C	38.36207658982351	-28.06433696690697	7.64774645695418
C	35.73531590440200	-28.92040983690839	2.23311763270144
C	31.34789351225903	-24.18926169267541	4.84704208175157
C	35.24180470082847	-24.59470261142381	9.50912706802856
C	38.51075760134717	-28.67128438351120	6.43256837998092
C	34.52519237372647	-28.41048165769933	1.85040104177361
C	32.46622990924616	-24.62233173173400	5.67459811910316
C	35.57983838565801	-25.58191483244587	8.49257922628824
C	37.34881933378206	-28.28598211173875	5.63779103212715
C	34.06237480847788	-27.58318148028685	2.96063405121608
N	36.52817410812983	-27.47204225253443	6.35574450013141
Fe	34.78256504128912	-26.64188020196048	5.75155937099155
C	32.58103117089632	-31.35215442381827	5.53571090090183
C	32.69938088564574	-32.35378220575448	6.67825620306610
C	32.48911406142702	-27.67782812961855	7.31795778988902
C	33.71991620853574	-27.96238050817069	6.48986799153240
C	33.83919581025979	-29.40083807342264	6.15501855352998
O	34.84373576916747	-30.05438811991320	5.96964605854265
O	32.58545346953886	-30.00229228747235	6.00517253534111
H	29.64080174236754	-22.93605866414791	4.42418732174637
H	30.93354847150621	-22.11523312947851	5.30718960247477
H	29.88451653460860	-23.25954419250715	6.14446066578472
H	30.97794804556321	-24.74186602360476	1.61773030424850
H	29.93971214061071	-25.93259418731551	2.40229240001189
H	29.65714482133822	-24.20682029426444	2.66343127690632
H	33.57343464666164	-27.65555134019643	0.05953056497980
H	34.35617389073505	-29.22770774342824	-0.13940989503241
H	32.81476153371835	-29.10615175606226	0.71819664441471
H	36.27703268198627	-30.03701936059771	0.46683118148130
H	37.65829390466908	-29.38257587255026	1.35616458273923
H	36.79586599255143	-30.78969163235486	1.98050766032864
H	33.84412559105395	-22.49417943060101	10.63428732270666
H	32.36203455922534	-22.98349925570712	9.80312741428999
H	33.46998990631474	-21.84852021221536	9.03117768382635
H	37.02877922294966	-24.08819488238695	10.62103496257904
H	36.03388791050146	-25.32653894185946	11.38652738871515
H	40.11600209796794	-28.78437525933775	8.67754960985929
H	39.66350231973676	-27.12952957744359	9.10690017068473
H	38.73227707376248	-28.48896055862035	9.73700884661771
H	39.23188019037565	-30.55444622177181	5.65500606407383
H	40.12908323872918	-29.14738487671950	5.07859904711997

H	40.36904504838781	-29.73142406438026	6.73041547558099
H	35.51894947089554	-23.63598093989869	11.42362252329584
H	31.91512339110907	-32.18633227023984	7.42277893133689
H	32.60458042627010	-33.38028317864991	6.30428977882666
H	33.67010343828607	-32.25321719312102	7.16676845151946
H	33.39702220009954	-31.49003040191581	4.82228474590308
H	31.62694439858411	-31.46781545584039	5.01302036468313
H	32.48358993204135	-26.66479122033198	7.71155542896967
H	31.59175922289295	-27.80591954637442	6.69726220934577
H	32.37417403126176	-28.38065213727285	8.15615765991969
H	32.29259013026035	-26.88432887756019	2.03345693792630
H	37.25405764667006	-26.41191575625701	9.48762289413353
H	37.85798936746644	-29.36099628567283	3.88411115872040
H	32.18695064471594	-23.24620233937394	7.26648496010065
O	35.82684801600254	-25.27020426521336	4.94917115272228
H	35.48308532344353	-24.41848022812202	5.25658571903561

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B3LYP Scan/Hydroxide IPC Model/RKS/220 degrees Constrained Optimization

C	30.42118316398472	-25.00709852577603	2.59469318013691
C	36.04164600169969	-24.32996577320553	10.78383951154313
C	39.61752107623781	-29.57508942664174	5.98450452839271
C	33.73477231860017	-28.69168852444380	0.63413934915656
N	33.13506928535774	-25.65908525152068	5.10651277291413
N	34.73990314828457	-25.47334299426567	7.45314388249811
N	34.94167407072295	-27.65985515278361	4.03630369703411
C	32.88705239545484	-26.84791182589761	2.97837213003033
C	32.80866482985378	-24.06198618869422	6.92948045516217
C	36.70536743920479	-26.40209135239089	8.58042709739046
C	37.09618598298558	-28.75283043181459	4.38354243223743
C	30.40062194492713	-23.09020340798966	5.22132015750560
C	33.44985753014543	-22.71826571107347	9.65720721074480
C	39.30842611771862	-28.06223747779658	8.84958781075891
C	36.60883993011278	-29.91301123670159	1.54007118173766
C	32.48973049426044	-25.91125920814958	3.93016466355070
C	33.86653322985953	-24.46273726712025	7.74445416787305
C	37.15191281304956	-27.26440501713396	7.58295697674395
C	35.96275446401359	-28.46361285479427	3.62983491576965
C	31.35106957432134	-25.01509958743252	3.77271439115674
C	34.19059251147409	-23.86468792245134	9.03318004556068
C	38.39284540037944	-28.03063758138639	7.66108975457358
C	35.96757421519513	-28.99069213615154	2.29545819504664
C	31.34156672196150	-24.20711241426629	4.87827089676698
C	35.27904471875966	-24.54591896523122	9.50948410739801
C	38.52326898766735	-28.66526848562680	6.45822016498358
C	34.48810685556519	-28.47696948439531	1.91383253323834
C	32.46608288148266	-24.62971334470263	5.70291904508218
C	35.61253461395772	-25.54240895531582	8.50022928956982
C	37.35088042358002	-28.29513239524464	5.67112102629550
C	34.04081624245620	-27.62761588320541	3.01320707366140
N	36.54245063306174	-27.46259176252760	6.38154074031205
Fe	34.79026232082199	-26.64217477725110	5.78666625123187
C	32.68744677428385	-31.25800360715136	5.27786484787888
C	32.55496848348317	-32.31663706004424	6.36532729925260
C	32.49233931712630	-27.68357784243900	7.35551691970472
C	33.73626580507763	-27.95239216457036	6.54346763464386
C	33.86956867107101	-29.38812929464309	6.20622318228715
O	34.87089439228334	-30.07065878732443	6.19303207238188
O	32.64691243888154	-29.93166656520848	5.81340129726965
H	29.62844871881558	-22.96258453527041	4.45412108536454
H	30.92547715130922	-22.12920563089911	5.31900494789240
H	29.88508093651104	-23.26672125991329	6.17600704510242
H	30.95330974209107	-24.79887019522092	1.65572671659934
H	29.91679826044213	-25.97495272215076	2.46422419860077
H	29.64157249642322	-24.24472941802289	2.70283024824137
H	33.52998312789950	-27.74366213432913	0.11744780182343
H	34.29634245511034	-29.32632693969150	-0.06064539138045
H	32.76256572590864	-29.17532024917833	0.80620071737324

H	36.21456771616873	-30.14039571654657	0.54307811201354
H	37.60863370336079	-29.47734835077726	1.40521120285822
H	36.74764045111299	-30.86960179378076	2.06318955610032
H	33.86963746011067	-22.45334132768465	10.63417060250867
H	32.38657348199055	-22.95138580980666	9.80989408278929
H	33.48874680702049	-21.81687718805818	9.02904634165237
H	37.06973501166404	-23.99059035722239	10.59258430198568
H	36.11912656266379	-25.25286089376566	11.37528169646660
H	40.16130337215149	-28.72903449449841	8.68077769016445
H	39.71193159298625	-27.06703127533197	9.08524162966219
H	38.79150405437364	-28.41586269740598	9.75288430610863
H	39.23048121019869	-30.56707826117742	5.71342142890886
H	40.12250493309644	-29.17506268977208	5.09375044582917
H	40.38316008569640	-29.72247789072389	6.75489612861024
H	35.56134380329534	-23.57609548181084	11.41761959293627
H	31.64276696659897	-32.16119980170666	6.94931169667480
H	32.51349461672319	-33.31936179149806	5.92334271154634
H	33.41184069940105	-32.27391757209108	7.03995063531282
H	33.61815166683609	-31.39316184836671	4.72289385209002
H	31.84690653448447	-31.30654252887212	4.57963161162749
H	32.46218174212963	-26.66702555622510	7.74014363319687
H	31.60665066273769	-27.83700819366589	6.72419035550961
H	32.38461074352535	-28.38024123786613	8.20091433860409
H	32.26823651539451	-26.93215153083175	2.08936946046552
H	37.30599162227239	-26.34570815453569	9.48402825757424
H	37.83305338181169	-29.41490768816529	3.93797869747021
H	32.19132654952343	-23.24233174860220	7.28613479296668
O	35.82574660526032	-25.28160153600824	4.95111358982940
H	35.47427376653501	-24.42524039676273	5.23600833144376

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B3LYP Scan/Hydroxide IPC Model/RKS/230 degrees Constrained Optimization

C	30.40851406228159	-24.99479867431988	2.61224903412929
C	36.06780892332815	-24.29551879235024	10.77282810880526
C	39.57171099186342	-29.62711445332046	6.00955337934380
C	33.68017101713970	-28.72490475786486	0.66987616727686
N	33.12576352033991	-25.64979835202762	5.12007298864529
N	34.74383445463074	-25.45441688712542	7.45604535608335
N	34.91474901948854	-27.67243025900860	4.05556463524178
C	32.86341356778302	-26.84936216428657	2.99957013814644
C	32.81265442548906	-24.04224296153648	6.93618771241535
C	36.71310419612269	-26.38244778323628	8.57735040531935
C	37.05678420906916	-28.78868739846767	4.40717222861654
C	30.40496104714254	-23.06589071693122	5.22997799410679
C	33.47102772516450	-22.68618089369991	9.65362352194223
C	39.29622113052666	-28.07214273680424	8.85568372119721
C	36.54185228936323	-29.97429074307141	1.57654106533133
C	32.47561076847251	-25.90434061529612	3.94678628262814
C	33.87393696851380	-24.44130047774709	7.74752824473060
C	37.14849882766357	-27.25695664521571	7.58542055237859
C	35.92392241091888	-28.49407062706693	3.65374717150695
C	31.34137144409468	-25.00258159355655	3.78790967573838
C	34.20682924988692	-23.83663566985968	9.03108013734470
C	38.37894469593080	-28.03951016838369	7.66859202830639
C	35.64565332846247	-29.03285690994145	2.32669711507135
C	31.33869836273563	-24.18973989006232	4.88979071221966
C	35.29748749732797	-24.51652300958065	9.50396634497523
C	38.49521065132434	-28.69191860720863	6.47397434020063
C	34.44139270073534	-28.50655687504975	1.94439710099383
C	32.46349682259185	-24.61442449708935	5.71330258869248
C	35.62298229442417	-25.51924093733407	8.49794587508780
C	37.32536798873218	-28.31452610850260	5.68635592730204
C	34.00976306195140	-27.63993343533826	3.03613245821654
N	36.53253454217685	-27.46023087925105	6.38844423658062
Fe	34.78180603094668	-26.63428052786460	5.79795921901279
C	32.86019788146817	-31.21708358421189	5.13692434888234
C	32.60304269333268	-32.29233509549757	6.18543943243599
C	32.49936483680509	-27.69081084222566	7.39811345671179

C	33.73798298335989	-27.93620081153619	6.57327139774294
C	33.90258096316359	-29.37426709563700	6.25738625365062
O	34.88751641721470	-30.06523705891217	6.39954002588089
O	32.75066158920500	-29.89706515474784	5.68281809382918
H	29.63048236057189	-22.93858687281253	4.46504601320062
H	30.93520543632352	-22.10709005377041	5.32004138413799
H	29.89215704706607	-23.23401644421376	6.18766382898482
H	30.93931179129253	-24.79338720386158	1.67104823144530
H	29.89871879014576	-25.96054558550888	2.48721091136035
H	29.63312316218866	-24.22791237384033	2.71897938963371
H	33.49121806454094	-27.78045267434405	0.14068223072410
H	34.22769446508311	-29.37928810648706	-0.01773508964357
H	32.69965003774159	-29.18775538906581	0.85144158557940
H	36.13786652851243	-30.21004790507709	0.58538945811233
H	37.54513446840119	-29.55099286809855	1.42882682981695
H	36.67507407643713	-30.92593862735135	2.11015231643060
H	33.90014720684814	-22.41327410998692	10.62432864757127
H	32.40950402112211	-22.91914845656347	9.81859214031610
H	33.50263850178010	-21.78964407891924	9.01818545677690
H	37.09747102884918	-23.96566558766451	10.57374278635000
H	36.14131256863197	-25.21389047866134	11.37188082600129
H	40.14214284424127	-28.74856182263063	8.69018439902969
H	39.70981443804865	-27.07946797239978	9.08429373069470
H	38.77703134214435	-28.41488701997486	9.76191255952187
H	39.16729361722587	-30.61833222670112	5.76176942229710
H	40.07506009743266	-29.25271002257849	5.10686593658919
H	40.34143848242572	-29.77084763798063	6.77654647376233
H	35.59616144399481	-23.53265341364611	11.40235033078294
H	31.62574046494316	-32.15008220402446	6.65672867598583
H	32.62198092556818	-33.28842597960367	5.72727006184902
H	33.37212274182401	-32.25393333179819	6.95836573490912
H	33.85144420706749	-31.34066265345206	4.69583479256372
H	32.11042508419324	-31.25441920864743	4.34199677101819
H	32.38051674666278	-26.64547070093040	7.67245089316436
H	31.61064639449312	-28.00846247057830	6.83611967646155
H	32.50355018636895	-28.29049817087277	8.32281249181897
H	32.24067575634474	-26.93455214387446	2.11335442315764
H	37.31828929082100	-26.32311954532481	9.47773927090688
H	37.78217242904640	-29.46756335497042	3.96801898274618
H	32.19952960332099	-23.21878002725305	7.29139909714083
O	35.81979530833110	-25.28600172608027	4.94437661533209
H	35.46494260176672	-24.42566040228363	5.21261257874831

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B3LYP Scan/Hydroxide IPC Model/RKS/240 degrees Constrained Optimization

C	30.39687680246496	-25.01272832238321	2.63762632209226
C	36.11093823180998	-24.25849763690485	10.75490864896196
C	39.56649269986255	-29.64939363456935	6.02060815143257
C	33.66948607321294	-28.73473231132381	0.68592084847976
N	33.12691839388886	-25.65528997293780	5.13505600862802
N	34.75798915329019	-25.44750946699128	7.46006886988335
N	34.90691072532093	-27.69011628624176	4.07318986488359
C	32.86169399219451	-26.85513854116736	3.01501504792650
C	32.81379295494661	-24.04895498634845	6.95191767290414
C	36.74362722216213	-26.35755268190385	8.56773452884540
C	37.03636694140715	-28.82887889842502	4.43154608595352
C	30.38955615870572	-23.08926239555009	5.25939217215917
C	33.48916752693187	-22.67604494827923	9.65637065260765
C	39.33162898281299	-28.03983580499427	8.83952654203143
C	36.51268390363240	-30.01734430332792	1.60314641212705
C	32.47426695846310	-25.91159559697521	3.96347013741088
C	33.88472873290863	-24.43838363969394	7.75522449207795
C	37.16767393877913	-27.24590862091169	7.58333431436359
C	35.90634358253091	-28.52637013943099	3.67636272094586
C	31.33436217027887	-25.01596101916421	3.80962248448540
C	34.22702741076078	-23.82409486633133	9.03180119221961
C	38.39777137475645	-28.02909992978705	7.66497605951047
C	35.62443265356578	-29.06604611567388	2.35041159091686

C	31.33001108625323	-24.20559120171530	4.91315195801826
C	35.32830859126344	-24.49264605731450	9.49592825688052
C	38.49658163272411	-28.70521163253251	6.48207814610748
C	34.42808308729068	-28.52510086586977	1.96359375075222
C	32.46094151416312	-24.62435148170347	5.73164162548638
C	35.64916569629386	-25.49962051562012	8.49259287543558
C	37.31811786570911	-28.33865326207125	5.70208782016067
C	34.00387977374388	-27.65149098700409	3.05271047919055
N	36.53654837379241	-27.46827371820791	6.39758234117481
Fe	34.78552993314923	-26.63853885303531	5.80995707679169
C	32.95891777568312	-31.18175665562656	5.04309378144789
C	32.44676701433617	-32.22837654831285	6.02424354812232
C	32.51491105258754	-27.69646457058863	7.43758801949575
C	33.74247308381276	-27.93187346276556	6.59518980469361
C	33.90848309513549	-29.37302760689121	6.29383944924314
O	34.84120663939196	-30.09112566660213	6.57974402126585
O	32.83183200489329	-29.85365710738219	5.56766747918399
H	29.60975119456423	-22.96757588187992	4.49895998807645
H	30.91266915404830	-22.12632716994544	5.34717962877748
H	29.88361433396944	-23.26215328089349	6.21987858527613
H	30.92215831922552	-24.80454507087682	1.69478482738464
H	29.89467241850285	-25.98236263163297	2.51211572104651
H	29.61563008488040	-24.25253362093285	2.74943252461721
H	33.49679885938166	-27.78854918457262	0.15425195897329
H	34.21070772543634	-29.39808145977262	0.00192774283832
H	32.68137826319629	-29.18281280303253	0.86334032730423
H	36.10748966980459	-30.25153435708854	0.61212149301603
H	37.51985714494240	-29.60338788954930	1.45529693209706
H	36.63725186409790	-30.96923391802938	2.13852065756808
H	33.92515544156085	-22.39637789869622	10.62208920103441
H	32.43080146760084	-22.91556958710917	9.83188291831664
H	33.50883722227409	-21.78181435533296	9.01721642315210
H	37.13463781415995	-23.91830716955215	10.54278472446506
H	36.20116130765973	-25.17368881781107	11.35648218489015
H	40.17695063358723	-28.71688401371215	8.67355769754447
H	39.74571117295273	-27.04244159559074	9.04535657169236
H	38.82626639193347	-28.36846218502270	9.75869013993159
H	39.15955993456257	-30.64586104681455	5.79921654078019
H	40.05585592451312	-29.29310920560502	5.10303231631054
H	40.34782511436119	-29.77680413249572	6.77867494903982
H	35.63835521271092	-23.49825941801863	11.38692286645104
H	31.41570996022807	-32.01247259019187	6.31950141902575
H	32.47214051492577	-33.22616031654616	5.57024841875743
H	33.06989524570232	-32.24284085440200	6.92040079254553
H	34.00459454318114	-31.36891204240077	4.79208864000222
H	32.36726173895008	-31.17847320894410	4.12410123137643
H	32.37775543892216	-26.64910643420866	7.69583781883941
H	31.62205700759932	-28.04437403153032	6.89901626116732
H	32.55402867781897	-28.27936269968596	8.37234173481194
H	32.23822093644929	-26.93917830005340	2.12918477757258
H	37.35957140790585	-26.28564769138713	9.45987405826062
H	37.75410724240488	-29.51851184088114	3.99649758393597
H	32.19825991920978	-23.22842604118128	7.30977091295256
O	35.82315133108006	-25.30011224842707	4.93871372501185
H	35.47256371378430	-24.43682823663249	5.20308379285891

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B3LYP Scan/Hydroxide IPC Model/RKS/250 degrees Constrained Optimization

C	30.40120369333194	-24.97694369414916	2.62946504170728
C	36.11259844057627	-24.26264231362328	10.75167345174949
C	39.54443321905358	-29.67026499716436	6.01287666578825
C	33.64854962392184	-28.72238975939545	0.67999905151400
N	33.12322664365860	-25.64077143072670	5.13031024933306
N	34.75525792450929	-25.44093676681925	7.45473987443818
N	34.90004949616810	-27.67487246970173	4.06103830966424
C	32.86189209341524	-26.82558755358030	3.00155645356892
C	32.80158722843004	-24.05131100603669	6.96096922397064
C	36.75115516128368	-26.34474272299395	8.54942077547584

C	37.01132612594275	-28.84528722037697	4.42849636158114
C	30.37927591083347	-23.08221290100517	5.27234120700823
C	33.47257162528744	-22.69631700935104	9.67625931129101
C	39.33633004180318	-28.03134757267051	8.81689713299641
C	36.47004719289969	-30.04431670589497	1.60769948773099
C	32.47470947318301	-25.88625891007121	3.95415928675956
C	33.87558733850779	-24.44094578107783	7.76020261823429
C	37.17055866010661	-27.23540273916047	7.56531326412043
C	35.88526082508308	-28.53089666369360	3.67133152420306
C	31.33440866115256	-24.99031272984046	3.80477275210691
C	34.21796077102437	-23.83284801487669	9.03978222656144
C	38.39651638281624	-28.02485620547086	7.64711406935837
C	35.59601079612526	-29.07506611128088	2.34855357103465
C	31.32410162165857	-24.19192839671943	4.91693786052122
C	35.32743477669879	-24.49447831739614	9.49389518036383
C	38.48410145956127	-28.71366139430470	6.47068760380992
C	34.40929147127638	-28.51694191747708	1.95706590816063
C	32.45322308897687	-24.61670370879585	5.73480975999449
C	35.65185746674538	-25.49243480295502	8.48252156563618
C	37.30438477542979	-28.34583966967093	5.69328685269542
C	33.99757458194647	-27.63081800991571	3.04100370868732
N	36.53282697302676	-27.46254991542589	6.38384032422572
Fe	34.78291786047691	-26.62616254188987	5.79951599474369
C	33.16881939619274	-31.24853156793986	5.08542801298789
C	32.40004572101041	-32.19032930076125	6.00315809965446
C	32.50920283411411	-27.70770428612604	7.41245311841156
C	33.74915073637549	-27.92539185044803	6.58399936749254
C	33.95993435327049	-29.37340493720172	6.35045822077271
O	34.83269507130154	-30.07251621882235	6.81701776840237
O	33.00887954896425	-29.88148637553214	5.48843101384341
H	29.60163371413001	-22.95427119153153	4.51071932320760
H	30.89927726041351	-22.11883182893461	5.37276030805555
H	29.87061123069719	-23.26731830793453	6.22912482359695
H	30.92985170268990	-24.75951069512871	1.69061488855056
H	29.90032830104357	-25.94580855340450	2.49288527603811
H	29.61883930632251	-24.21852695454141	2.74546184621647
H	33.49268811498465	-27.77708601213660	0.14149277540219
H	34.17906254244739	-29.39961130272434	0.00122837273504
H	32.65268669167529	-29.15199888599990	0.85941435255473
H	36.06106957765777	-30.27949624817367	0.61845484042494
H	37.48306752561955	-29.64599959941639	1.45647419433145
H	36.58140669348001	-30.99435722234266	2.14925169369653
H	33.90462729070340	-22.42612728376157	10.64644408800522
H	32.41511453830919	-22.94370677286873	9.84616902257802
H	33.48895098850828	-21.79410266556579	9.04825264887129
H	37.12989440255144	-23.90391947331828	10.53910923488935
H	36.21962219223042	-25.18333618892592	11.34185922409720
H	40.17763712905029	-28.71359619541898	8.65173543510157
H	39.75609857670648	-27.03445268640631	9.01330434739909
H	38.83399030832114	-28.35101023409529	9.74083089824154
H	39.12923867650353	-30.66637788598338	5.80533320304762
H	40.03039354726612	-29.32779863615307	5.08825978067108
H	40.32966086586774	-29.79476156821868	6.76736662342310
H	35.63114867490975	-23.51738004366886	11.39476819738258
H	31.34478547165464	-31.90638092037357	6.05514195079757
H	32.45958717326319	-33.22214021079510	5.63722919613369
H	32.81654909345706	-32.16031974266816	7.01228262906335
H	34.23136059250226	-31.49731334974619	5.07924978663659
H	32.78619777416491	-31.28966302131298	4.06274713349295
H	32.34135854635954	-26.66032276540934	7.65242982300148
H	31.62968292902998	-28.08617347978901	6.87055591440247
H	32.55650805409514	-28.27609567240873	8.35561086374549
H	32.24003337834372	-26.90348789000027	2.11400911662296
H	37.37184774337835	-26.27088591993033	9.43811043284811
H	37.71881785133189	-29.54798182661849	3.99744164338332
H	32.18145672607736	-23.23743823520038	7.32601624005143
O	35.81957107543385	-25.28398350996348	4.93196843881967
H	35.45329382567815	-24.42259607178651	5.18070850388338

B3LYP Scan/Hydroxide IPC Model/RKS/260 degrees Constrained Optimization

C	30.39672836989638	-24.97406159079435	2.62821710415015
C	36.12492746380966	-24.24075353081590	10.73645848193035
C	39.52312451777851	-29.69470390983754	6.02619080796563
C	33.64832154975650	-28.71364372726644	0.67522628782829
N	33.11458710214586	-25.64340980224332	5.13197688172486
N	34.75113038495196	-25.43930027275883	7.45324951967231
N	34.89065283030764	-27.67816286916856	4.06337132806337
C	32.86007738777580	-26.81934387412443	2.99783278506687
C	32.79155491327553	-24.05616137572760	6.96418719298662
C	36.75342005557042	-26.33508245005108	8.54335394669654
C	36.98958796591536	-28.86838057236948	4.44106698371020
C	30.36434682403022	-23.09192753270989	5.28014402417814
C	33.47434443008763	-22.68681266481752	9.66902635169978
C	39.33531981848805	-28.02548418756629	8.81356961666252
C	36.45328014072398	-30.06040947960411	1.61735379648905
C	32.46933272542677	-25.88474240742818	3.95340634262237
C	33.87084654919013	-24.43968920178405	7.75920706533448
C	37.16603996216229	-27.23486684056864	7.56489681601943
C	35.86961397021133	-28.54341217140312	3.67894202676045
C	31.32730598573367	-24.99051818968492	3.80553625804096
C	34.21889620859165	-23.82464345758377	9.03379520674367
C	38.38920801198691	-28.02817315852392	7.64881849016668
C	35.58251689906324	-29.08549501435416	2.35466972726927
C	31.31268566397495	-24.19750356225012	4.92132685774900
C	35.33300433783209	-24.48092180374742	9.48444040770189
C	38.46811315906103	-28.73008111080392	6.47943239595865
C	34.40326908897881	-28.51634931395479	1.95697215143491
C	32.44196758557959	-24.62276085595304	5.73904983803253
C	35.65355424601121	-25.48347731843820	8.47649744787785
C	37.28701951110310	-28.36428180344129	5.70324413274206
C	33.99339682936613	-27.62750876936215	3.03956373434325
N	36.52194003693814	-27.47080671837092	6.38819058998169
Fe	34.77358098500313	-26.62947058963776	5.80053809991312
C	33.24969968399969	-31.24489116798010	5.04855128880420
C	32.40671840780558	-32.16593787547725	5.92076336322166
C	32.53891148037031	-27.71040174440601	7.47407028273508
C	33.74160836471296	-27.92607976120175	6.59207504661888
C	33.94416497096557	-29.37786146922453	6.37362643585042
O	34.73941239508357	-30.09217940453339	6.94577887298028
O	33.08149658929810	-29.86909733761561	5.42119688545018
H	29.58734182994391	-22.96295781685786	4.51804089830622
H	30.88152134176688	-22.12751827321928	5.38524770942759
H	29.85501574465688	-23.28244315187473	6.23551474885266
H	30.92698383854598	-24.75050699181899	1.69170171838676
H	29.89898449259766	-25.94367801258656	2.48566052453114
H	29.61197990947537	-24.21840958755226	2.74611344681186
H	33.50460240033053	-27.76645278074161	0.13665480681392
H	34.17655937937140	-29.39520440665744	-0.00098052324582
H	32.64741712641474	-29.13402990718556	0.84826881126342
H	36.04692060249859	-30.29286353941278	0.62640088672074
H	37.46943002812041	-29.66846958604223	1.47030646718944
H	36.55656000048592	-31.01131547560366	2.15900675249013
H	33.91141538652091	-22.41071692317146	10.63529320793093
H	32.41854730878107	-22.93601230074002	9.84639076986692
H	33.48468722822174	-21.78771633550266	9.03645316080895
H	37.14002722465931	-23.88041138648054	10.51622609980961
H	36.23775206455576	-25.15816494883401	11.33063494941310
H	40.17386974656817	-28.71170291371357	8.65086272865134
H	39.75886321347797	-27.02778841356515	8.99730634486382
H	38.83724109710973	-28.33420647239223	9.74348601433494
H	39.10404603341079	-30.69154363817909	5.83007879166824
H	40.00605411980639	-29.36275274994206	5.09617200772626
H	40.31130413915206	-29.81435490013529	6.77836498049793
H	35.64522106454367	-23.49348623928696	11.37853504904123
H	31.35469336074297	-31.86661301736622	5.89774493792410

H	32.47570152195878	-33.20218695461009	5.56949064234816
H	32.75471055259995	-32.13041520492772	6.95505642172363
H	34.30702145444622	-31.50633574959387	5.11799254769668
H	32.93940981038629	-31.29163670736342	4.00216873111182
H	32.37112087022695	-26.66226994158164	7.71096062608882
H	31.63634586706681	-28.10319160173540	6.98066398309242
H	32.64124757778370	-28.26941939633333	8.41805571244513
H	32.24143386341526	-26.89319550271371	2.10768960761318
H	37.37889165866147	-26.25484009163080	9.42811009378740
H	37.69180980509989	-29.57850675737129	4.01352846147612
H	32.17022609822035	-23.24361343202269	7.33016972674857
O	35.81092061890119	-25.29035972056088	4.92773032363774
H	35.46332336951030	-24.42750382610816	5.19738230096717

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B3LYP Scan/Hydroxide IPC Model/RKS/270 degrees Constrained Optimization

C	30.39586049914963	-24.90698834587036	2.61183081787318
C	36.11672133183644	-24.25835647163158	10.73166378051451
C	39.45784677184758	-29.74564607495785	6.01758737628381
C	33.59998757763402	-28.68852937218229	0.66214879444241
N	33.09648032603637	-25.61973775868861	5.12253699871811
N	34.73189655168647	-25.43787986615274	7.44641450260617
N	34.85892436231416	-27.66021671248728	4.04631525905381
C	32.83480474013221	-26.78408784801001	2.98316200092637
C	32.78671485352847	-24.03442969765975	6.95896206221356
C	36.72554384086846	-26.35497465899131	8.53487765403715
C	36.94053382628238	-28.87968115283618	4.42625955811919
C	30.37757356412020	-23.03420484098350	5.27074890028308
C	33.47978678579674	-22.67884086321452	9.66764535436036
C	39.28434449822131	-28.07991988608100	8.80876525933144
C	36.39525728679146	-30.05919340725146	1.59994903002656
C	32.45186099401937	-25.84854232948388	3.94117622861994
C	33.86086730215496	-24.43120722998686	7.75440946721813
C	37.13022474468405	-27.25691071611787	7.55537034203859
C	35.82729613841143	-28.53623259316119	3.66203681885104
C	31.32128031816876	-24.94007550212964	3.79284060665615
C	34.21430061308730	-23.82201774523590	9.03034094682591
C	38.34276794511730	-28.06611770781422	7.64057441711863
C	35.53433734677925	-29.07576122992249	2.33764173101511
C	31.31273814847233	-24.15084346331020	4.91143316055028
C	35.32250619695827	-24.48915545535156	9.47942128989938
C	38.41579737194109	-28.76665361252787	6.46987971561612
C	34.36039252659954	-28.49571561364189	1.94119856287551
C	32.43403421476872	-24.59268975752012	5.73099071529897
C	35.63392295496151	-25.49253939777197	8.46923316471191
C	37.24222122801429	-28.38320026045836	5.69104222680599
C	33.96074868882629	-27.60210865883568	3.02403187936291
N	36.48668136345478	-27.48178479445593	6.37594096325027
Fe	34.74695577013524	-26.62189504121405	5.78859931591937
C	33.53495307175375	-31.31629890307175	5.14073310894996
C	32.59399046152008	-32.20976761385309	5.93807773382705
C	32.50364974474827	-27.69802775104580	7.45079963207131
C	33.71694065185869	-27.91818998414048	6.58475968709794
C	33.97241605402137	-29.37288520346856	6.46000765124336
O	34.66957989473790	-30.04022427257638	7.19620305602588
O	33.29256233923869	-29.92588385839540	5.40442075963013
H	29.60516674330783	-22.89234085442224	4.50628537638829
H	30.90690077121727	-22.07702706773127	5.38119856937732
H	29.86214541448609	-23.22134134489554	6.22350832521690
H	30.93268627674348	-24.68524043307393	1.67863874003860
H	29.88721347214718	-25.86992767987875	2.46244292345786
H	29.61945885348002	-24.14278995682698	2.72998276316613
H	33.46004175646918	-27.74078861796545	0.12354012976686
H	34.12143692070471	-29.37373503638426	-0.01564819002758
H	32.59724368209715	-29.10264323585785	0.83965171888980
H	35.98318225039032	-30.29195977385118	0.61141682705705
H	37.41366224269425	-29.67514288848484	1.44746587470845
H	36.49399360372040	-31.00907432340948	2.14427119539385

H	33.91938362512629	-22.40817642926445	10.63430349970647
H	32.42187246515708	-22.91916046901387	9.84468097302378
H	33.49792171429716	-21.77877373102422	9.03660004792116
H	37.13514868432934	-23.90737527831265	10.51168673957739
H	36.22089054210462	-25.17759566691267	11.32457452319308
H	40.11584377225697	-28.77466608197604	8.64597857249467
H	39.71825979596483	-27.08794676953270	8.99903943850848
H	38.77876887720284	-28.38774737610831	9.73486829068237
H	39.02430469028163	-30.73546440471108	5.81692396877263
H	39.94921356546484	-29.41864160480502	5.09023946585128
H	40.24121717369034	-29.87974868466033	6.77227942204533
H	35.64416670753660	-23.50739272845651	11.37474143306085
H	31.55073831803598	-31.93923549739863	5.75014629352069
H	32.73076302610028	-33.26127630910938	5.65959712275991
H	32.79130844539942	-32.10931242153493	7.00704614523295
H	34.57696682339387	-31.54611545721943	5.37059343434431
H	33.37508475037713	-31.42561423209886	4.06576529256038
H	32.30465125780547	-26.64540324868775	7.63868818791309
H	31.61279076730209	-28.13832804469541	6.97468468248234
H	32.62121848435827	-28.21111894825954	8.41818071830863
H	32.21609586683476	-26.85015884784333	2.09242328319070
H	37.35002041985791	-26.28393171019248	9.42111687485125
H	37.63490312033382	-29.59670887858099	3.99728424461824
H	32.17359302246851	-23.21630932422145	7.32634971930662
O	35.79756096164214	-25.28457066632700	4.92882796921635
H	35.43378738754021	-24.42138386678123	5.17489421515398

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B3LYP Scan/Hydroxide IPC Model/RKS/280 degrees Constrained Optimization

C	30.38665412480243	-24.85429664881230	2.59833846973022
C	36.10343766995087	-24.29016795058024	10.72770619535028
C	39.39516033557645	-29.79640479503187	6.00108449193121
C	33.56409972308659	-28.65149485409685	0.63496889229855
N	33.08190029107838	-25.59634000003181	5.10619314262629
N	34.71570641174548	-25.43805037314350	7.43288918665250
N	34.82573793529141	-27.64842400099825	4.02583344486586
C	32.80896229453617	-26.75373871485969	2.96464665286262
C	32.78768360369425	-24.01161924493514	6.94593623238220
C	36.69291646861548	-26.38618570570777	8.52548758291238
C	36.89408423300522	-28.89088906016471	4.40407733328917
C	30.38763906157296	-22.98530527524824	5.26049799719162
C	33.48815862557976	-22.67536957088010	9.66258375939634
C	39.22793850491513	-28.14652650857549	8.80240491260247
C	36.35281480567771	-30.03986835428057	1.56629476549644
C	32.43428227463697	-25.81704913001245	3.92495693511325
C	33.85566769659987	-24.42285895963353	7.74235296934284
C	37.08917064429976	-27.29086881774924	7.54502959296944
C	35.78831402822239	-28.52857868221822	3.63807161529873
C	31.31243132256627	-24.89757725275337	3.77869067254895
C	34.21236122942462	-23.82319886635893	9.02194431714800
C	38.29145129415048	-28.11498209148545	7.63059347145827
C	35.49481195791249	-29.05792496611671	2.30955647087780
C	31.31239880313666	-24.10965709018638	4.89830038525320
C	35.31096420623438	-24.50544876481882	9.47169388311295
C	38.36134826624767	-28.80979152575572	6.45603508964199
C	34.32467902054799	-28.46954541190118	1.91529487464285
C	32.42981638797197	-24.56344838198518	5.71647897398662
C	35.61350046232720	-25.50856619144877	8.45836045456947
C	37.19561472892185	-28.40832030617109	5.67471949080637
C	33.92924228659876	-27.57955123798117	3.00292110333081
N	36.44735765493202	-27.50251582249302	6.36209948654258
Fe	34.71900847127607	-26.61798229537519	5.77202457529450
C	33.80579912357589	-31.36401908559156	5.27757510234332
C	32.78371800882171	-32.25228064673100	5.97428117875747
C	32.46928985135324	-27.66556642882094	7.44250578957974
C	33.68202521249943	-27.90229903646622	6.58024844797181
C	33.98233085961633	-29.35335238275025	6.55332158865718
O	34.56615139508220	-29.96549503035282	7.42548572654378

O	33.49336850921649	-29.97102198319840	5.43469852927585
H	29.61602466269520	-22.83499146106966	4.49688413189699
H	30.92553267282635	-22.03313011281094	5.37263242388382
H	29.87121055268394	-23.16994689854478	6.21318374911546
H	30.92480472709807	-24.63521197973176	1.66527089490157
H	29.86990920250449	-25.81266691379145	2.44733595198061
H	29.61661547616779	-24.08397573364012	2.71834195563611
H	33.42860325000252	-27.70014404598966	0.10159875942310
H	34.08267071957837	-29.33524556544006	-0.04649944118856
H	32.55947015745731	-29.06220174078880	0.80988799739973
H	35.93811878286898	-30.26869759881366	0.57793711041302
H	37.37129981205251	-29.65630816732671	1.41271288739508
H	36.45225715184292	-30.99192370093748	2.10672563129182
H	33.92879796966370	-22.41295402467828	10.63103416666969
H	32.42768763422154	-22.90627410043500	9.83695482415016
H	33.51602817737918	-21.77298855579357	9.03522429287889
H	37.12749696347677	-23.95279217418656	10.5126600936907
H	36.19248723517280	-25.21291460087385	11.31761449119230
H	40.05305136696813	-28.84859326441090	8.63839840898781
H	39.67117103780732	-27.16037358075636	9.00113863902614
H	38.71500010973463	-28.45551151535594	9.72400056197259
H	38.95259507775510	-30.77982037229863	5.78863996483671
H	39.89552376324921	-29.46657626632440	5.07954875539111
H	40.17253958368013	-29.94592187132380	6.75901238436243
H	35.63903327343294	-23.53493834131839	11.37171764909429
H	31.77220075811774	-32.02546240563436	5.62466430927615
H	32.98807571699534	-33.30966105139051	5.76926361986010
H	32.82128360612111	-32.09883877486052	7.05431304624182
H	34.80987726283409	-31.55000066829347	5.66288339845714
H	33.80196343785515	-31.52521877941750	4.19734693578825
H	32.23524096358486	-26.61027521785673	7.56136131846277
H	31.58697606107939	-28.17027566918719	7.01558637820888
H	32.62275283772658	-28.10694315193282	8.43912996629724
H	32.18991759735115	-26.81222606119054	2.07358018005549
H	37.31442294724597	-26.32685523246656	9.41465823390835
H	37.58356934695962	-29.61040753960411	3.97127832657576
H	32.18288116003484	-23.18807966395799	7.31496380671117
O	35.79158119989424	-25.29121653036276	4.92286928894935
H	35.41823911157837	-24.42543876450201	5.14426054847161

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B3LYP Scan/Hydroxide IPC Model/RKS/290 degrees Constrained Optimization

C	30.38490792471256	-24.69901551605829	2.57314719404043
C	36.05616510728459	-24.42710267665234	10.74998202202085
C	39.28572575092817	-29.87038770459225	5.91220725833663
C	33.45230219427214	-28.57952893597564	0.58075513525410
N	33.07459139029385	-25.52654506621637	5.06101194985494
N	34.67984933234484	-25.46246791309939	7.41490419168024
N	34.74826033838132	-27.62098790543214	3.97156393783202
C	32.75234070112614	-26.67095655449867	2.91941804360147
C	32.81253492214557	-23.96122434288667	6.92427646810146
C	36.61203272460148	-26.49328528286500	8.51079973305878
C	36.79624227991044	-28.90250828176238	4.33010600748803
C	30.45554195812511	-22.84016842403335	5.24227055032177
C	33.50875221316221	-22.70723661606617	9.68099718979598
C	39.11720100014609	-28.29789884647270	8.75857607516699
C	36.22171239380872	-30.01863201727104	1.48571285481031
C	32.41261763711616	-25.72363119518210	3.88276438552284
C	33.84989021487477	-24.42674037001593	7.73078415344169
C	36.99440320417813	-27.38796528018819	7.51523612649468
C	35.69595874499802	-28.51182425191888	3.57148389343381
C	31.31822619512494	-24.77097742529140	3.74601650534604
C	34.20709043038239	-23.86368214267493	9.02750419156666
C	38.18505189405779	-28.22871352309811	7.58492301894841
C	35.38890139635755	-29.02294702151380	2.23879715792471
C	31.34773648489492	-23.98714973701879	4.86861328773399
C	35.27574157062286	-24.59005646644995	9.47887757812434
C	38.25340264963484	-28.89332194255885	6.39180244150982

C	34.22637381419540	-28.41422608282414	1.85503475055160
C	32.45304559798535	-24.47838639170343	5.68045468408791
C	35.56000988347567	-25.58326091593186	8.44970859997392
C	37.09582307166226	-28.45956122856466	5.61603205701723
C	33.85058319226301	-27.52635857833102	2.95138857712115
N	36.35272185164369	-27.56521671101431	6.32605886698009
Fe	34.66297795905692	-26.61329760340503	5.73450998157305
C	34.44688174140460	-31.39667240882154	5.82906955133304
C	33.32062740281774	-32.36041769819300	6.17669952457004
C	32.23058603746242	-27.62123109766323	7.16780024473445
C	33.57517824482001	-27.86402003251675	6.53288937859251
C	33.98845084125409	-29.26433213017796	6.79548661595111
O	34.31468532397059	-29.69451888367568	7.88565196290275
O	33.95813985601816	-30.05464186003241	5.68279309579086
H	29.68444909946060	-22.66460640346656	4.48367503033230
H	31.01939251991462	-21.90355843336726	5.35749062886389
H	29.93919649900072	-23.01706791957339	6.19636895272989
H	30.92005015692034	-24.48699818738997	1.63670463275138
H	29.84520040638290	-25.64452448081381	2.42137249979157
H	29.63321160546501	-23.91248151506838	2.70373663587430
H	33.31712853310108	-27.62288185869361	0.05692140989065
H	33.95939242266984	-29.26079270178179	-0.11166992621941
H	32.44681672016053	-28.98564540845395	0.76229208251882
H	35.80606308359358	-30.22036241430578	0.49188620128167
H	37.25227411614581	-29.66414819023663	1.34352726854429
H	36.28877059870713	-30.98188967467277	2.01151781865194
H	33.95127841972064	-22.46903593324268	10.65483236868168
H	32.44205730013211	-22.91434415263479	9.84769576572388
H	33.56174465132303	-21.79734058768228	9.06626149925402
H	37.10038826866709	-24.14452161080023	10.55407350906470
H	36.08513466140300	-25.35754529529096	11.33379727993364
H	39.93753577388564	-29.00216936551232	8.58045268410346
H	39.56749236943181	-27.32047224973946	8.98245687267966
H	38.59791112980502	-28.62464059098167	9.67034975213037
H	38.84076738911386	-30.84202658316901	5.65517487254311
H	39.8000920207654	-29.50828244825079	5.01066515337845
H	40.05211770342774	-30.05450330500715	6.67359402468034
H	35.62253284515699	-23.65210216942141	11.39200674869400
H	32.51165127931837	-32.28832292299678	5.44389358364359
H	33.68549559983133	-33.39416987359390	6.18462057268207
H	32.91524394346408	-32.13195119268595	7.16481128525400
H	35.22370745756699	-31.41245160211012	6.59494680906764
H	34.89186921106792	-31.63805440373694	4.86119645864278
H	31.92776725436778	-26.57768331021043	7.13422026809111
H	31.45455082604871	-28.21883233270659	6.66094194900253
H	32.24127415613732	-27.95771512626103	8.21473994908325
H	32.12733463577285	-26.71003454227044	2.03143295412665
H	37.22629491462789	-26.46821013817121	9.40655738452523
H	37.48024587990157	-29.61745537639121	3.88105042204986
H	32.23066801840382	-23.12458494017455	7.30050118317020
O	35.81273996832379	-25.31771499778097	4.93753781061909
H	35.36188506098620	-24.46136424170450	4.97655570357272

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B3LYP Scan/Hydroxide IPC Model/RKS/300 degrees Constrained Optimization

C	30.36190215589186	-24.70815367230969	2.58937886834026
C	36.05673911965540	-24.44367164143061	10.75011559003796
C	39.28295700907330	-29.86235784241214	5.89512895090440
C	33.42187218366355	-28.59362872893379	0.58916977388868
N	33.06553973500910	-25.52988321486087	5.06345276076252
N	34.67061634917781	-25.47444620588904	7.41781614680462
N	34.72590922599615	-27.63201039079603	3.97591362813469
C	32.72233256217597	-26.68908414839760	2.93322694755497
C	32.82874626560648	-23.94602489021027	6.91435562988924
C	36.58552581651227	-26.52806604475094	8.52298612317347
C	36.78779962437297	-28.89523013120481	4.31983002930671
C	30.47080005440783	-22.81990961572609	5.23679402755663
C	33.54404697211724	-22.68329053408650	9.66243778394139

C	39.09426191984897	-28.32966081882282	8.76160221829296
C	36.21241645276416	-30.00407266281313	1.47405780510997
C	32.39323067194190	-25.73369274497043	3.89236838709720
C	33.85858453344883	-24.42184991964285	7.72480109639532
C	36.96645816946253	-27.42158430568724	7.52552973182286
C	35.68173475550827	-28.50985608130644	3.56729650561483
C	31.30495307633501	-24.77408334040183	3.75475485021455
C	34.22296386163758	-23.85662714106376	9.01857335327539
C	38.16203306284566	-28.25577526332189	7.58821417959979
C	35.37373638465749	-29.01872143357535	2.23405908153826
C	31.35071009594355	-23.97791310866762	4.86804524509787
C	35.27627761345308	-24.60013228668080	9.47817461093403
C	38.23880349102669	-28.90346181055332	6.38600526635343
C	34.20154078767362	-28.42310251040353	1.85931875958731
C	32.45784996917426	-24.47026195331325	5.67679491581015
C	35.54562854862734	-25.60452092967596	8.45599122951917
C	37.07935318797615	-28.46931727810184	5.61316508228776
C	33.82289952514357	-27.54198473655156	2.96042272118953
N	36.32655178113625	-27.59176853327243	6.33396633792058
Fe	34.64238922505999	-26.62891035838480	5.74145721020625
C	34.55960800796139	-31.36738199893306	5.88021752106089
C	33.42532618371716	-32.36081234066224	6.08932359539894
C	32.20893154910132	-27.58029596961702	7.19742769471605
C	33.53487483685056	-27.86578633536276	6.54044832330785
C	33.92092755603048	-29.27147053933987	6.81855852783549
O	34.09048582054363	-29.73149682585023	7.93424372420343
O	34.06484983751214	-30.03292964038224	5.69763720823082
H	29.69691130949636	-22.64424632339464	4.48112376646299
H	31.04337234890373	-21.88730591977871	5.34066145122931
H	29.95847019907679	-22.98427235886791	6.19527695220898
H	30.89021234664236	-24.51168941928205	1.64571917619965
H	29.81333271994785	-25.65103459624883	2.45389080441748
H	29.61762261772707	-23.91419236021909	2.71734121973940
H	33.26541500881176	-27.63585170214580	0.07354885249288
H	33.93680024851428	-29.26026839083196	-0.11166974435357
H	32.42536986609202	-29.01984211069464	0.77431732527020
H	35.79917799451253	-30.19977235429744	0.47801584990310
H	37.24146494005951	-29.64365427930509	1.33634049009796
H	36.28294530049892	-30.97131267170787	1.99219721211679
H	34.00029816585536	-22.43526224662763	10.62743653601925
H	32.47726687240302	-22.87675970174608	9.84455315160306
H	33.59924581166546	-21.78360472426730	9.03322742801916
H	37.11264728491514	-24.20994255949728	10.55324861715025
H	36.04419502273416	-25.36185954542358	11.35383230476320
H	39.91316507089583	-29.03515144687689	8.58176087676146
H	39.54678057496011	-27.35363870452599	8.98739457509127
H	38.57479458872970	-28.65704841514024	9.67299840749914
H	38.84886828092331	-30.83290654704877	5.61656143439214
H	39.79988411478816	-29.47835920945288	5.00420166397107
H	40.04598594930120	-30.05384673615496	6.65806843698264
H	35.65348429392563	-23.63753953916983	11.37332790898880
H	32.70000958613191	-32.29673062440536	5.27292205027581
H	33.81309100994553	-33.38572866102135	6.12378827294212
H	32.90948870245858	-32.15656786923903	7.02990769905399
H	35.24972252845358	-31.38002108836951	6.72535209108023
H	35.11292036710704	-31.58363341630315	4.96382597960034
H	31.95023575564081	-26.52482744563976	7.18891321953046
H	31.40167787828022	-28.13009406737347	6.68489740024415
H	32.21636121409728	-27.94282056778006	8.23442794131988
H	32.09151997041642	-26.73145744834558	2.04951232268328
H	37.19795658402853	-26.50772932228593	9.42011151687358
H	37.48038456167743	-29.59604919947976	3.86169150053889
H	32.25895078337841	-23.09860473725359	7.28479888230303
O	35.80534552604796	-25.34364781815265	4.94531744008480
H	35.36736577491402	-24.48108148627838	4.99239688552661

C	30.34438780322482	-24.71979909334079	2.59079634489170
C	36.04067246361407	-24.46110777833339	10.74967866039805
C	39.27904843000843	-29.85846810486614	5.88264750247632
C	33.39837866051852	-28.61160599921403	0.59286459623980
N	33.05597223833683	-25.53516571835436	5.05789822273949
N	34.66239046584135	-25.47993497548144	7.41043993537167
N	34.71210047045836	-27.63913235973878	3.97269550659290
C	32.69920533079584	-26.70767655481767	2.93780603565170
C	32.83689614141819	-23.93527227381377	6.89708128450968
C	36.56364662476115	-26.54950949018099	8.52429144980057
C	36.78775229040267	-28.88352438496031	4.30411189958532
C	30.48071940085542	-22.80620598442592	5.21880071272580
C	33.55536678647624	-22.67297181736902	9.64465592372271
C	39.06983326419799	-28.35560575361454	8.76396469245310
C	36.20924676522962	-29.99300087247599	1.46065536791999
C	32.37664570342051	-25.74553556604012	3.89231296930926
C	33.86078965616067	-24.41752693854157	7.71137430516394
C	36.94848153164687	-27.43819449455957	7.52368825375900
C	35.67543076528309	-28.50560428528432	3.55740134660134
C	31.29313016884494	-24.78080902570147	3.75176861138854
C	34.22479895582400	-23.85453259423661	9.00600907641651
C	38.14512816184988	-28.27100218162099	7.58529369362384
C	35.36506349803675	-29.01610234410802	2.22536406169773
C	31.35030376143331	-23.97414571359440	4.85684165840411
C	35.26616419355518	-24.61022980853719	9.47321867097295
C	38.23072016249440	-28.90571981896007	6.37656550637918
C	34.18384895844004	-28.43363379126401	1.85841973781137
C	32.45810517748973	-24.46648055028620	5.66486413015551
C	35.53051665655862	-25.61839573288400	8.45352187250613
C	37.07418972366564	-28.46744530469221	5.60174229079032
C	33.80321615009180	-27.55633256199015	2.96198754834039
N	36.31477521499138	-27.60031922773350	6.32747299194232
Fe	34.62996073582482	-26.63752550221454	5.73499953349863
C	34.64047692969790	-31.34872848066771	5.93417242788450
C	33.48866188790153	-32.34011543284466	6.03230350041824
C	32.23691553948310	-27.54216881455734	7.26951707692232
C	35.52362331065997	-27.86562819089752	6.55340740298905
C	33.892326885769469	-29.27624106155757	6.84104763976790
O	33.93747888478384	-29.76826654575559	7.95681975965712
O	34.17028565822922	-30.01037067268142	5.72795628515285
H	29.70402802540840	-22.63243978447009	4.46560516512544
H	31.06066959768910	-21.87685714100817	5.31019537034268
H	29.97248761018323	-22.95736464405872	6.18158823288965
H	30.86945431438279	-24.53903493359365	1.64222885561793
H	29.78664318589906	-25.65918128252707	2.46914628727817
H	29.60799407777199	-23.91770512541910	2.71345388647123
H	33.23937682579270	-27.65694159775278	0.07211981938473
H	33.91035487748437	-29.28232733757421	-0.10621264216381
H	32.40286016490318	-29.03679282930667	0.78513230368860
H	35.78753532263443	-30.19998612047110	0.47046308600450
H	37.23140321050408	-29.61866122288473	1.30924863836346
H	36.29934283807119	-30.95593661108736	1.98358850043134
H	34.00086334643306	-22.43635191771114	10.61748648591870
H	32.48306468153650	-22.85019810651687	9.80963922724608
H	33.63449474125502	-21.77146670388268	9.02049372373581
H	37.09595284132547	-24.21834292224528	10.55990977167481
H	36.03132643911137	-25.38540485374100	11.34379773941285
H	39.89306291601439	-29.05514637863720	8.58077758376614
H	39.51636890129229	-27.38054711841804	9.00519717636387
H	38.54566448892378	-28.69672251210396	9.66766004265014
H	38.84840647641869	-30.82859234205596	5.59723189316249
H	39.79684634236536	-29.46754490669843	4.99529547751199
H	40.04078494038009	-30.05228595675298	6.64629010793044
H	35.62963073802710	-23.66393662113881	11.37930376155992
H	32.83994116442290	-32.26746218114254	5.15448540254713
H	33.86855731013137	-33.36672143652165	6.09460940485181
H	32.89191468849429	-32.13927793478518	6.92423550987566
H	35.25571634050452	-31.37899249415274	6.83525557258251

H	35.26878732161082	-31.55520891898643	5.06507707106510
H	31.97869192281352	-26.48809931744984	7.22228833363035
H	31.39811824511281	-28.11659250908624	6.84175962320890
H	32.30927510174087	-27.85111112030794	8.32065160151136
H	32.06376171158373	-26.75520734707074	2.05767706422220
H	37.17099409153445	-26.53555536655323	9.42497859535682
H	37.48611884587036	-29.57466804913680	3.84004260417185
H	32.27528652617581	-23.08017468244323	7.26228001612564
O	35.79640045256595	-25.35605867248321	4.94034727443740
H	35.37607314642865	-24.48664874062652	5.01451228741419

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B3LYP Scan/Hydroxide IPC Model/RKS/320 degrees Constrained Optimization

C	30.32405675117380	-24.74545410986239	2.60500308280965
C	36.03740241275126	-24.46983009370488	10.75009247098251
C	39.29029155097753	-29.84208380728245	5.87174957157440
C	33.38666451972096	-28.62765153120613	0.60021940521453
N	33.05144480250417	-25.54462310300047	5.05952889139956
N	34.66211664342073	-25.48491408731894	7.40853578455514
N	34.70335585430706	-27.65038748703850	3.97741778744609
C	32.68117616109224	-26.73128184520462	2.94993474381408
C	32.84911006883173	-23.92851681943697	6.88636124530693
C	36.55286451305881	-26.56537474062198	8.52985827546508
C	36.79367125334349	-28.87334936521205	4.29684287301308
C	30.48674179464552	-22.80569909009120	5.2125505050032
C	33.57423727379865	-22.66034289053829	9.62985299021878
C	39.06429315882462	-28.36532694750602	8.76519847995525
C	36.21790109346258	-29.97791499293661	1.45173954757760
C	32.36366671710487	-25.76377187767242	3.90064265145488
C	33.86980430350476	-24.41361958008442	7.70306875657982
C	36.93997569483713	-27.45104196139447	7.52724259349503
C	35.67513633689204	-28.50416491424408	3.55543625231563
C	31.28155077237850	-24.79754243329262	3.75918438404697
C	34.23490881424861	-23.84988878079723	8.99695851876189
C	38.14108659152628	-28.27799863246619	7.58550888828714
C	35.36488248362091	-29.01410428807722	2.22323713800014
C	31.34972582880570	-23.98005782488455	4.85557760658835
C	35.26642858154749	-24.61490866634425	9.47101058600290
C	38.23386528291073	-28.90131222883041	6.37135731228811
C	34.17489731880556	-28.44512318719842	1.86342823910802
C	32.46159671571576	-24.46830660616548	5.66056702758457
C	35.52532588809999	-25.62825532372812	8.45518213763227
C	37.07585031414225	-28.46468935866399	5.59769265106886
C	33.78980754595512	-27.57419277109723	2.97059000701988
N	36.30931932998232	-27.60908775028796	6.32891110586351
Fe	34.62288002087534	-26.64889393357512	5.73739501199940
C	34.67424847824451	-31.34223998298221	5.97203642699884
C	33.49851310213862	-32.31075646101139	5.94405796068523
C	32.25855677972596	-27.50484528832195	7.32509416781050
C	33.51212057983358	-27.86820147511460	6.56853496887007
C	33.84152228749286	-29.29112675328203	6.84951703557096
O	33.73803721640532	-29.83158221920272	7.94052966094277
O	34.25558103410182	-29.98959316638700	5.75615871560073
H	29.70566500969145	-22.63608643042193	4.46299052618693
H	31.07063765423707	-21.87769514828914	5.29142928470476
H	29.98449784571996	-22.94632998398946	6.18003640473094
H	30.84215932679541	-24.57532953045011	1.65066075116027
H	29.76323255824986	-25.68464822829583	2.49703196424364
H	29.59048207397361	-23.94046114908924	2.72543516374640
H	33.21850879028615	-27.67361497162872	0.08121294520486
H	33.90173648043938	-29.29345534080274	-0.10126657208327
H	32.39518758663692	-29.06094685837208	0.79511646869874
H	35.79307522194109	-30.18930134558884	0.46381664565807
H	37.23372480564036	-29.58896756336983	1.29470050387971
H	36.32461429567779	-30.94008169493706	1.97286355820487
H	34.01723926587158	-22.42628215945721	10.60442268747439
H	32.49949600112176	-22.82684594778813	9.78983820882770
H	33.66528390242362	-21.76086199728688	9.00439363128650

H	37.09524881027831	-24.23561419271259	10.56380516236890
H	36.01867781527450	-25.39311985957111	11.34551329062543
H	39.89093646637303	-29.06008445500551	8.57927227363114
H	39.50607567229171	-27.38968506189607	9.01279367954969
H	38.54042081647925	-28.71388722611360	9.66626017752041
H	38.86768749064951	-30.81325862568213	5.57807656781489
H	39.80633895507820	-29.44015428289022	4.98831791245139
H	40.05237310630520	-30.03591967784794	6.63504644596088
H	35.63035964651677	-23.66855431170365	11.37708236052502
H	32.93665880665029	-32.20750768699951	5.01124544034501
H	33.85167047315115	-33.34593936613496	6.02070044531410
H	32.82651269469070	-32.11237918857650	6.78074882470068
H	35.20728221422765	-31.40858356671655	6.92265300221290
H	35.37168553075709	-31.54431062638884	5.15608994180076
H	32.02019146891397	-26.44722654622563	7.26713430945557
H	31.39237330565314	-28.07000179097330	6.94238653088455
H	32.36158705717600	-27.79608007397778	8.37807674814481
H	32.04099718440750	-26.78443906333956	2.07359746408318
H	37.15770896441732	-26.55437602679108	9.43226400053389
H	37.49874377470039	-29.55378204444218	3.82707524434855
H	32.29417775518196	-23.06695642378396	7.24648064488947
O	35.79147205589172	-25.37257459372355	4.93980046038272
H	35.38557239841860	-24.49818412566881	5.03339073812197

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B3LYP Scan/Hydroxide IPC Model/RKS/330 degrees Constrained Optimization

C	30.31125791877416	-24.75365088614189	2.61988424360516
C	36.03569485751295	-24.48265289185959	10.75578918864684
C	39.30358294280865	-29.81685122059111	5.85216815159555
C	33.35159435598986	-28.65587299058155	0.62179993532117
N	33.04511278530650	-25.55320491420621	5.06696759772235
N	34.66131835958753	-25.49185870034703	7.41231589738942
N	34.68208184809351	-27.67080072150784	3.99117260493349
C	32.65285030115902	-26.75761974612969	2.97179893047260
C	32.86578268545893	-23.91877204311944	6.88003194064335
C	36.54400867493941	-26.58188655162314	8.53720309429284
C	36.78985678276759	-28.86773046564972	4.29236381034939
C	30.51240862517992	-22.78398343994749	5.20234942458210
C	33.59578359163340	-22.64985707679414	9.62181855337829
C	39.06666678150792	-28.36821051552369	8.75848656089005
C	36.20270729308957	-29.97784829407081	1.45051967328211
C	32.34799060112506	-25.77870060803316	3.91496265451751
C	33.87946869726168	-24.41127715413107	7.70088779953740
C	36.93283818106503	-27.46230948919070	7.53027396175107
C	35.66028763877608	-28.51323784552680	3.56083590988289
C	31.27517501740388	-24.80279957229541	3.76881728906007
C	34.24639068874859	-23.84774062849422	8.99428017989084
C	38.14072434377750	-28.28034748618461	7.58098888160900
C	35.34512537044189	-29.02498967042943	2.23056312318883
C	31.35947530748859	-23.97270826324197	4.85461140742704
C	35.26765857889188	-24.62269985055379	9.47440156558468
C	38.23790028612906	-28.89153366807297	6.36108451249828
C	34.14623705028420	-28.46840542486261	1.88032567685983
C	32.47012603982780	-24.46404578485756	5.65925461520730
C	35.52036486329126	-25.64060399260239	8.46161740894651
C	37.07387242446431	-28.46024141655482	5.59312132162596
C	33.76164063010285	-27.60066061615428	2.99009902273979
N	36.30186168787677	-27.61707852631697	6.33222489588947
Fe	34.61215327976649	-26.66319024968110	5.74688327173813
C	34.73422997168982	-31.33666487375204	6.07894360115341
C	33.57552712908522	-32.28490528033438	5.79543237523096
C	32.24612045270877	-27.47589023241854	7.34184807199424
C	33.49380210771437	-27.87279515883753	6.59024707570977
C	33.77072135987051	-29.30860007967711	6.87183882821293
O	33.47989419592695	-29.89253115361464	7.90735199695339
O	34.37430299896364	-29.97146900859415	5.84663137500000
H	29.72981335632736	-22.61334932246325	4.45465470724907
H	31.10791939217482	-21.86237069479152	5.26788199200283

H	30.01323298231536	-22.90775199606638	6.17368333777845
H	30.82523904310363	-24.59944449108594	1.66062661198570
H	29.74016194710946	-25.68811050260497	2.52583904514329
H	29.58671468208538	-23.93986878827371	2.73576541468074
H	33.17488085618081	-27.70277797711242	0.10388944663664
H	33.86653529525792	-29.31858014622982	-0.08267084801495
H	32.36383207069992	-29.09493891046386	0.82233385987172
H	35.77315710857039	-30.19071284102215	0.46495005605211
H	37.21314791437812	-29.57758192090178	1.28746020183229
H	36.32308301249837	-30.94025030041442	1.96805851416888
H	34.03726917930038	-22.41831100766338	10.59765831904836
H	32.51875642244391	-22.80485189813037	9.77769638623618
H	33.69880943616425	-21.75276915852718	8.99476818267531
H	37.09667288154996	-24.26054147174021	10.57251081155459
H	36.00484661096102	-25.40412315390751	11.35351931217651
H	39.89736235813274	-29.05666939873635	8.56732264776335
H	39.50262515180160	-27.39112962375952	9.01070349905332
H	38.54687401529912	-28.72488040580653	9.65878502055496
H	38.89218650434790	-30.79142462727953	5.55382147906081
H	39.81190123190505	-29.40333928712061	4.96961846190941
H	40.07043243433624	-30.00621363170614	6.61179130844048
H	35.63532442913989	-23.67533857338970	11.37930507546701
H	33.19373423082509	-32.13203580363324	4.78198785642061
H	33.90091515053581	-33.32792922796477	5.88752712738070
H	32.76367206485374	-32.11372144596985	6.50446000503613
H	35.08230056174830	-31.45024329658620	7.10768974860508
H	35.56704393395672	-31.51823263400872	5.39565516599168
H	32.01707359580592	-26.41872439380575	7.25450888025197
H	31.37299843686332	-28.04590082222843	6.98489319089188
H	32.34948735182520	-27.73478789304081	8.40308171652369
H	32.00660999531573	-26.81556079783434	2.10024444986152
H	37.14830251135841	-26.57378656641515	9.44000659466542
H	37.50087818523926	-29.53701232445921	3.81552939408193
H	32.32086387476441	-23.04837536726118	7.23405990122589
O	35.77988540461997	-25.39482291862981	4.93786500044955
H	35.37576883271278	-24.51889343305960	5.02462103797267

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B3LYP Scan/Hydroxide IPC Model/RKS/340 degrees Constrained Optimization

C	30.28619103067452	-24.80595199287011	2.65307325965739
C	36.05471615804873	-24.45437511720421	10.75301389511533
C	39.32253434855410	-29.79765554285098	5.86616043759090
C	33.33510243055142	-28.70515803692559	0.66209583728215
N	33.0439420387983	-25.56967106065991	5.08423826325302
N	34.67121566289838	-25.48662639295495	7.42034468453585
N	34.67651417198925	-27.69390795680665	4.01930228486150
C	32.63547296458879	-26.79991804196310	3.00721450660305
C	32.88157072335670	-23.91075093294658	6.87650483743787
C	36.55143347500108	-26.57407834344687	8.55169200820478
C	36.79781048321434	-28.86864597184448	4.31232829301391
C	30.51294444256669	-22.79881003842751	5.20479553881434
C	33.62509981091463	-22.61708599323403	9.60365444477898
C	39.08284770114029	-28.34826068248411	8.77138610244406
C	36.20755910316787	-29.99084409774770	1.47573781999186
C	32.33657338063335	-25.81105324012393	3.94171253804713
C	33.89621345427194	-24.39823692006791	7.69925547530643
C	36.93925041925444	-27.45841650298438	7.54757340298818
C	35.66085635421268	-28.52778854103487	3.58592071486719
C	31.26194348866495	-24.83754477546782	3.79257986842170
C	34.26809469679170	-23.82449812986623	8.98653406179623
C	38.15228102829537	-28.26928292828959	7.59683587430787
C	35.34262512434157	-29.04772919925954	2.25974287283647
C	31.35719765905622	-23.99182090933718	4.86521245993083
C	35.28472098118112	-24.60150135832940	9.47353823020786
C	38.25084019770397	-28.88034032776664	6.37714809518398
C	34.13476707580666	-28.50599946047048	1.91570640565250
C	32.47524665630046	-24.47226037195894	5.66647376097984
C	35.53052712789471	-25.63031950419084	8.47033835198302

C	37.08183849391926	-28.45768367331539	5.61177406994367
C	33.74917538907247	-27.63680612868815	3.02392686092122
N	36.30632816998771	-27.61877241493450	6.35180510568020
Fe	34.61294796015908	-26.67318843608902	5.76585757500820
C	34.69770594508383	-31.34256616177284	6.07339441202184
C	33.58026898870380	-32.21419165448688	5.51255951547531
C	32.27303844757667	-27.44065082254913	7.41086413595062
C	33.48786799800229	-27.87147998078281	6.62331850622235
C	33.68419294875355	-29.33120509103686	6.84853451250159
O	33.22210144944621	-29.97056722547223	7.78580175321444
O	34.42635146260990	-29.95163023979752	5.88945415040561
H	29.72415233029153	-22.63786550934383	4.46150380778686
H	31.10887669805338	-21.87644556326344	5.25349499891280
H	30.02195310752715	-22.91032660018902	6.18174435934165
H	30.78991972969021	-24.66374686259131	1.68654695635353
H	29.71643634442257	-25.74288059624360	2.57779631266383
H	29.56094792563355	-23.99230429036409	2.76532405999977
H	33.14937397890622	-27.75578474175520	0.14052799784203
H	33.85130504373625	-29.36773845497812	-0.04156468440007
H	32.35148235570117	-29.15009323929341	0.86953792640564
H	35.77378398619395	-30.21207931357988	0.49387576540407
H	37.21084423804038	-29.57638137913034	1.30420652992901
H	36.34570205168651	-30.95004439343772	1.99456312108100
H	34.07132079375064	-22.37727287991407	10.57532994217336
H	32.54802710181519	-22.76573311924992	9.76518459216483
H	33.72970072517595	-21.72723659761973	8.96669675871243
H	37.11778391066358	-24.24522317700512	10.56676339247625
H	36.01492887717728	-25.36846563463036	11.36154573326908
H	39.91551711384350	-29.03431833390999	8.58017282360825
H	39.51601694898121	-27.36837890261500	9.01757640436457
H	38.56822959508804	-28.70286019950113	9.67548978602957
H	38.91839537828260	-30.77542936266595	5.56836424448230
H	39.82617572369160	-29.38015186866475	4.98279299843429
H	40.09227654498134	-29.98111366973283	6.62432462174481
H	35.66289411822309	-23.63586426046679	11.36727199811017
H	33.38791069099197	-31.96189577551132	4.46598421306170
H	33.85438968650972	-33.27453926253595	5.56654673350009
H	32.66142472510490	-32.06562623926444	6.08271760922827
H	34.84964672079010	-31.54641223792040	7.13548962590332
H	35.63380912722364	-31.51283156959821	5.53614738096317
H	32.06214778675591	-26.38042152760459	7.31912240617861
H	31.37817536074584	-27.99963399154485	7.09616277259631
H	32.40509582853983	-27.68540607257421	8.47282052522383
H	31.98265065659874	-26.86864023482626	2.14140450887307
H	37.15806986283304	-26.56034223450387	9.45287861659731
H	37.51309094827958	-29.53218923080060	3.83386730395684
H	32.34124804756403	-23.03426868720705	7.22237331173454
O	35.77705622819708	-25.41342084918247	4.94130118519746
H	35.39623225303743	-24.53094247934025	5.06100777865598

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B3LYP Scan/Hydroxide IPC Model/RKS/350 degrees Constrained Optimization

C	30.25876081529090	-24.85997287976829	2.70085827712604
C	36.09293275756536	-24.40703574318024	10.74769608615161
C	39.34200058218395	-29.77851874272051	5.88818022963910
C	33.30524713333331	-28.76893248932003	0.72412761392456
N	33.03960317487700	-25.58994729829003	5.11569524408343
N	34.68310676535206	-25.48310608777421	7.43967986278031
N	34.66832475743630	-27.72323328035450	4.06141766804043
C	32.61175306704659	-26.85100242684755	3.06123704395138
C	32.89930689469117	-23.90367054285402	6.88293434968725
C	36.56554687868112	-26.56177156957988	8.57483786531953
C	36.80419684473966	-28.87223153786438	4.34406747362008
C	30.51878402075396	-22.81010367345417	5.21522311215097
C	33.67093476049007	-22.57024247858904	9.58232589258386
C	39.10443929154407	-28.32576664488310	8.79141072746580
C	36.20373074527497	-30.01352374050280	1.51510851504980
C	32.32103754001473	-25.84871141020642	3.98410414457945

C	33.91685114657164	-24.38478754416801	7.70589852721476
C	36.95006477485953	-27.45207820030232	7.57451298799411
C	35.65793789324717	-28.54824969918272	3.62416347637850
C	31.24661480002110	-24.87532625044559	3.83020505248948
C	34.30032476381467	-23.79321681617122	8.98164891793225
C	38.16805539065289	-28.25590234166748	7.62089922256782
C	35.33242065513623	-29.08048269173500	2.30457480674205
C	31.35560313711456	-24.01153715811169	4.88705824680016
C	35.31375779261106	-24.57012834049540	9.47567987668306
C	38.26609431680121	-28.86749773054996	6.40159591345662
C	34.11388724818474	-28.55551989836378	1.96974450464025
C	32.47995865880878	-24.48208991346095	5.68528910979469
C	35.54715070112216	-25.61588877134233	8.48731210669073
C	37.09111914742099	-28.45390545380374	5.64019883416368
C	33.73046814087036	-27.68201013350108	3.07537417450999
N	36.31359045932486	-27.61851567601448	6.38217671504084
Fe	34.61452925445555	-26.68737216773566	5.80057484834115
C	34.65433750584056	-31.35768195252770	6.06101515435005
C	33.64252372192056	-32.10120865430782	5.19688197055535
C	32.25923936589837	-27.43130006376263	7.42627836813468
C	33.47523906364474	-27.88067050030328	6.65115708210508
C	33.57018326139484	-29.36300959040029	6.77903540108683
O	32.90062220487333	-30.05368119326578	7.53980335637182
O	34.49417537523836	-29.94209471422369	5.96282908372188
H	29.72490178947693	-22.65679563200801	4.47577050065468
H	31.11889186930633	-21.88966495752609	5.24551276947252
H	30.03506094234862	-22.90502981153751	6.19754309498191
H	30.75169029949239	-24.72929301516209	1.72715413374392
H	29.68986952125537	-25.79864496512203	2.64398878583945
H	29.53334987859530	-24.04612626143856	2.81063167755951
H	33.11924322126559	-27.82604168829952	0.19089269553402
H	33.81448455333230	-29.44291644721253	0.02629131813586
H	32.32169340709932	-29.20744134721293	0.94441201732269
H	35.75832171465146	-30.25318721398390	0.54282995723153
H	37.19495062936204	-29.57961740608284	1.32276170293726
H	36.37093195762181	-30.96423536583806	2.04069161961926
H	34.13328663926326	-22.31107271027253	10.54142264693428
H	32.59599736890702	-22.71090631916769	9.76403766406139
H	33.76879334266719	-21.69507638081323	8.92443810183907
H	37.15891099582347	-24.22440468871391	10.55102101088199
H	36.03811028870427	-25.30428971924544	11.37991712599275
H	39.93449274074820	-29.01563858594830	8.60252174016735
H	39.54142756986108	-27.34466112675224	9.02606389791517
H	38.59397206926929	-28.67031022446565	9.70171040252706
H	38.94228429082135	-30.75729208520302	5.58789469732949
H	39.84394989204294	-29.35658397521192	5.00590908232900
H	40.11253487830145	-29.96032348652806	6.64594697429022
H	35.72099560669677	-23.56539774837680	11.34276756265153
H	33.68193972593900	-31.73654215143001	4.16676890076269
H	33.85438495957453	-33.17711786758437	5.19413141394020
H	32.63245670861261	-31.94997149475039	5.58210940313375
H	34.56766883684868	-31.66364619565520	7.10638407616733
H	35.67421072226836	-31.54156238851537	5.71446801952994
H	32.11717725211465	-26.35609097859132	7.40710373770255
H	31.34739736038917	-27.91047099496493	7.03974164505138
H	32.32923643650690	-27.75837899443633	8.47257771170794
H	31.94967122832857	-26.93373898930498	2.20373002881177
H	37.17633947593218	-26.54023497653352	9.47309568874705
H	37.52310658421014	-29.53083478287625	3.86428117471401
H	32.36626198497495	-23.01918154405064	7.21955361144461
O	35.76330744250342	-25.43686826700446	4.94355260945887
H	35.39915015877886	-24.55006675314744	5.08185829695639

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B3LYP Scan/Hydroxide IPC Model/Triplet/0 degrees Constrained Optimization

C	30.58475715732076	-24.76653069180636	2.36979205511964
C	35.56076604156297	-24.51094846663674	10.98102471993687
C	39.26514561818796	-29.83109340327458	6.35525072503575

C	33.80322844845935	-28.72769687202315	0.64280447085585
N	33.18134799502263	-25.53520197820614	4.96838304415167
N	34.59744311461120	-25.48205446704726	7.48826146123580
N	34.86514602506306	-27.62122951637808	4.06836077142875
C	32.90171417453639	-26.77524605077351	2.88177947869106
C	32.90510608233204	-23.87389353997291	6.74952400490030
C	36.28896835962724	-26.62232880800629	8.82885565451162
C	36.94453182573114	-28.80969549458750	4.57647057072180
C	30.66829563712495	-22.75022620135186	4.92302617783205
C	33.36834219817401	-22.58654397166995	9.53548727204536
C	38.73702124107944	-28.47701708939860	9.26752313932063
C	36.61147603641506	-29.97055017327937	1.72177233413397
C	32.54190728657838	-25.77913136424199	3.78701329204749
C	33.82489525325683	-24.37280582381121	7.66938252182471
C	36.77030446363034	-27.48203481567156	7.84614667781741
C	35.88327441067570	-28.46844011205688	3.74277817450106
C	31.48845331766742	-24.79880830709910	3.56747221887652
C	34.04734172492532	-23.81169155070745	8.99774008902295
C	37.94931636954076	-28.32680819400476	7.99948455089786
C	35.67837854122651	-29.01636930816890	2.40845419953555
C	31.52694515018527	-23.94779934322408	4.64069691638488
C	34.96612758351179	-24.62171951866411	9.60813952132604
C	38.17002783082584	-28.89608074298105	6.77573751009478
C	34.49764985849020	-28.49241168206970	1.95193105629223
C	32.58800970724980	-24.43225384025569	5.51285380676758
C	35.30966258868617	-25.65202677631794	8.63626410344594
C	37.10441329629295	-28.41714259049692	5.90173249026415
C	34.01559105447878	-27.60309290998111	2.99969333969777
N	36.27630015074822	-27.57621579925671	6.58060482200403
Fe	34.69773251838053	-26.59569233043052	5.79899074866717
C	34.53741404448894	-31.33121771427200	6.04406183179989
C	33.77316381132619	-31.94032670737968	4.87211109546583
C	32.04730116934989	-27.35420911746842	7.16463640913807
C	33.32562802305617	-27.89487939003408	6.57173599560213
C	33.33507401136777	-29.34243019535446	6.59250130229598
O	32.44563006587445	-30.08437725373305	7.02451185397317
O	34.47408159486328	-29.91018372084487	6.05019204119686
H	29.94250078077146	-22.57481706391923	4.12113523437663
H	31.26676674572362	-21.83479775355255	5.02964140565276
H	30.10067437293188	-22.86847481702220	5.85655920223870
H	31.14980870100355	-24.65193166005822	1.43401067833507
H	29.99950312464287	-25.69194119985021	2.27543787437190
H	29.87332266096481	-23.93521805826941	2.42459845230750
H	33.64715615412579	-27.79147150883900	0.08874653869250
H	34.38091068990823	-29.39677164653645	-0.00454035413438
H	32.81291885109145	-29.18293388004992	0.78270809613128
H	36.27106285909772	-30.20538369898519	0.70728865183433
H	37.62635486982958	-29.55724016562866	1.64011442330747
H	36.69815755985467	-30.92094414245441	2.26636337639609
H	33.71534814601480	-22.34655248526482	10.54664871322041
H	32.27751388166006	-22.71211199077912	9.58528690248983
H	33.55856327041896	-21.70691956590355	8.90492616129075
H	36.65061714289863	-24.37417422267921	10.94311366216211
H	35.37501958632115	-25.41347504415770	11.57994063484379
H	39.58341578870306	-29.15999083451455	9.13557028250660
H	39.14194747710266	-27.51589698644995	9.61452925141825
H	38.11988264510027	-28.87569131358860	10.08506873071502
H	38.86931437155380	-30.79684389447369	6.01123713720568
H	39.85555975779315	-29.41596166400450	5.52645787319949
H	39.95806573752358	-30.03832893125447	7.17842921708802
H	35.14338603017504	-23.66182124367594	11.53327245889548
H	34.11723711149254	-31.51144405513710	3.92680147416566
H	33.92057108907692	-33.02723092980851	4.83678769211779
H	32.70640064451279	-31.73812851303490	4.97780887478766
H	34.15290018287331	-31.72329097718698	6.98993000655867
H	35.60465955905980	-31.56125880390128	5.97056248271433
H	31.32764121702631	-27.10930751557275	6.36773939146707
H	31.55642611776047	-28.08329504915536	7.81653325899969

H	32.20899151404224	-26.42763094544606	7.71792090107168
H	32.31133596784557	-26.86074855240860	1.97435920896715
H	36.77952245622554	-26.64938256075335	9.79747455662894
H	37.68990997638252	-29.48832373122679	4.17156240564855
H	32.34866518415376	-22.98857327666162	7.04345365743270
O	35.90228201514270	-25.33172902207203	5.12492976800944
H	35.65478798126888	-25.15158304278492	4.20534416602406

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B3LYP Scan/Hydroxide IPC Model/Triplet/10 degrees Constrained Optimization

C	30.58065915457969	-24.81424047258402	2.35179095024862
C	35.56114693740662	-24.45217107218187	10.95910980502419
C	39.26525682882696	-29.82569467000593	6.39653844030321
C	33.82438519271904	-28.76073652402834	0.65572831053521
N	33.16660241546399	-25.56101921207386	4.96831366367584
N	34.58310150751571	-25.47639475781953	7.48556629315648
N	34.86735165746943	-27.63868653605509	4.08177800937448
C	32.90003619979860	-26.81240031635072	2.88737245464358
C	32.88925643023438	-23.87812601045431	6.72932006657542
C	36.28154328382426	-26.59665652937574	8.83523378966982
C	36.95272666307565	-28.81248459510862	4.60016877034550
C	30.65942961534172	-22.77003313618860	4.88282501074020
C	33.35940784365904	-22.55292189219059	9.49395949448726
C	38.73024137583536	-28.44641718350882	9.29545150275797
C	36.63737251853115	-29.98253935042197	1.74817010000443
C	32.53175091111196	-25.81430425729080	3.78615668676836
C	33.80973181452390	-24.36636773828706	7.65403282344019
C	36.76631677216097	-27.46455962816149	7.86124527509625
C	35.89320647157214	-28.47821740606753	3.76135113056567
C	31.47979343375006	-24.83542260635168	3.55314140625071
C	34.03626850479725	-23.78642174469150	8.97275928556303
C	37.94576188741944	-28.30700618347860	8.02414502735108
C	35.69629059149903	-29.03162766551508	2.42826022246375
C	31.51528139337679	-23.97346813636998	4.61724152129299
C	34.95868321143666	-24.58640525182778	9.59162775674632
C	38.16973602201428	-28.88634364518860	6.80576379339796
C	34.51235662628657	-28.51869078147314	1.96715501592924
C	32.57252521546647	-24.45087263858135	5.49874577973747
C	35.29992513496497	-25.62986775352761	8.63315104952016
C	37.10603341126512	-28.41508767567978	5.92489293758372
C	34.02020066066558	-27.63103960130807	3.01176368636938
N	36.27501008800384	-27.57034918346792	6.59534141198888
Fe	34.69248076455597	-26.60475262696246	5.80622485092186
C	34.45100351068077	-31.34906828523252	5.86692977136636
C	33.66077530150091	-31.86369754044962	4.66743259460053
C	32.21932675271726	-27.38738380131952	7.46367317159645
C	33.35025982106525	-27.91473997548511	6.61480486591497
C	33.31893770586176	-29.36165183170959	6.55403730983298
O	32.41345088951461	-30.10166685004689	6.95452110206758
O	34.43122838020761	-29.92927516864252	5.95862322853351
H	29.93946517210076	-22.59958669420083	4.07463568034360
H	31.26117054164769	-21.85611144855476	4.98405395553154
H	30.08566128838645	-22.87639450160647	5.81405765342704
H	31.14942198229354	-24.71199066299534	1.41685886895712
H	29.99312800268546	-25.73904795209368	2.26603563317287
H	29.87148492751231	-23.98026364335315	2.39449043804563
H	33.67356065316012	-27.82772966000818	0.09469807798221
H	34.40387624486198	-29.43544014662836	0.01586684054513
H	32.83233119234774	-29.21268731535747	0.79321880947463
H	36.30566768216777	-30.21738106169570	0.73082240735216
H	37.65187917192021	-29.56692665768063	1.67526862820531
H	36.72115051228185	-30.93318602029475	2.29290141678637
H	33.70875373743015	-22.29773683664427	10.50060313509365
H	32.26859384904287	-22.67680702544494	9.54801855338953
H	33.54893396598877	-21.68298243536196	8.84985308440760
H	36.65064569839496	-24.31539941934342	10.91242104481332
H	35.37945444417564	-25.34397290609969	11.57510994301328
H	39.57529548913681	-29.13264276248310	9.17216177996504

H	39.13667913803733	-27.48281147982413	9.63381967241422
H	38.11038125132639	-28.83550310543233	10.11555290560942
H	38.86912710736609	-30.79309254074564	6.05757753816079
H	39.86010540643289	-29.41745262920825	5.56746401091732
H	39.95416144002198	-30.02819481697595	7.22425843244385
H	35.14658052594761	-23.59365394362633	11.49881846697572
H	34.01245644560994	-31.39104495592213	3.74622210432548
H	33.77363366673990	-32.95082076733264	4.56784911398968
H	32.60152575145782	-31.63529743359812	4.79378250706578
H	34.06050500200773	-31.78456893071169	6.79100542402493
H	35.51029227606625	-31.60637299075611	5.77133167176056
H	31.86530180411468	-26.41131916111536	7.12922365990655
H	31.37585320463739	-28.08446687868531	7.49657061169266
H	32.55658116991289	-27.25139044906858	8.50347136059416
H	32.31347417135873	-26.90567234795563	1.97828773876958
H	36.77284583570169	-26.61185093152630	9.80378314737571
H	37.70226686361401	-29.48954548570133	4.20037192273624
H	32.33355943347931	-22.98885733449490	7.01253990574843
O	35.88957615904833	-25.33964852827073	5.12250069196104
H	35.60678189488291	-25.12336448373748	4.22107969458026

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B3LYP Scan/Hydroxide IPC Model/Triplet/20 degrees Constrained Optimization

C	30.56654473964002	-24.82792030540237	2.36251135635964
C	35.57812453683569	-24.44225992936098	10.95080990403481
C	39.24408850075159	-29.85578269514346	6.40387490201704
C	33.82242809563554	-28.75692706517955	0.65302809629202
N	33.16490003739681	-25.56367249492044	4.96974826913149
N	34.58730878435244	-25.47546336436046	7.48386266134530
N	34.85592947607241	-27.65347095328930	4.08819461752278
C	32.89333568347328	-26.81830811421231	2.89137391179002
C	32.89215463393997	-23.87802632735691	6.72842843706744
C	36.28539503295966	-26.59680223847761	8.83343058717847
C	36.93920215364428	-28.83137831291263	4.60625799498595
C	30.65035725286661	-22.77921711504703	4.88994765856600
C	33.37450560175880	-22.54394331878369	9.48686703020921
C	38.72180021423254	-28.46273085373644	9.29842730440278
C	36.63293604352801	-29.98285668221977	1.74452041528849
C	32.52613240928815	-25.82015490940391	3.79039433188173
C	33.81608822507272	-24.36370180248750	7.65106410395872
C	36.76390682124943	-27.47083131184057	7.86198983227794
C	35.88155252726984	-28.49340021060065	3.76659346160037
C	31.47112827607134	-24.84395150403943	3.55981330677272
C	34.04783593534749	-23.78000632969759	8.96718844971808
C	37.93764574695489	-28.32121054638467	8.02722191288368
C	35.68868193442697	-29.03829055025212	2.42942510545313
C	31.50870663184301	-23.98035192888338	4.62241378415757
C	34.97086065839585	-24.57960028286706	9.58573906820036
C	38.15648637244325	-28.90627262420691	6.81085309378624
C	34.50673516494618	-28.52118330936347	1.96744999645369
C	32.57054468184539	-24.45413365493280	5.50063344564842
C	35.30707773191934	-25.62689740302276	8.62980990188322
C	37.09570248335172	-28.42992193218575	5.92918896911790
C	34.01230233701307	-27.63872151812307	3.01503119275190
N	36.27118712165229	-27.57691474995497	6.59682642444161
Fe	34.68984311713633	-26.60858717483554	5.80808643490931
C	34.42783668969608	-31.35186065981054	5.92406175182317
C	33.77590240782514	-31.79386543851675	4.61759200597345
C	32.22173035857108	-27.37596088943758	7.49263166445455
C	33.33410615176258	-27.90608590051141	6.62106395013321
C	33.27035906849508	-29.34870149359993	6.51522011563207
O	32.28813913807570	-30.06465548409612	6.73841076171977
O	34.44276116141733	-29.93635855146593	6.07675136163665
H	29.92840136571523	-22.61053005214418	4.08316821251553
H	31.24988478399496	-21.86374355289432	4.99019424650808
H	30.07863275585684	-22.88734375631329	5.82224043419400
H	31.13097573323850	-24.72830669030233	1.42465900490476
H	29.97985101944548	-25.75375885300512	2.28271879569834

H	29.85660155318808	-23.99462076220713	2.40548980086399
H	33.65936578075026	-27.81953204917713	0.10314649076858
H	34.41109080555992	-29.41630308242575	0.00559348049147
H	32.83657779466922	-29.22401241839636	0.78494399864614
H	36.30598077410627	-30.20750068923273	0.72335200376385
H	37.64755098797693	-29.56613662833183	1.68076150389303
H	36.71462414437239	-30.93923502071626	2.27945887820538
H	33.72709205620958	-22.28657847923128	10.49181989606032
H	32.28366705087322	-22.66608362717315	9.54433587374677
H	33.56351312786931	-21.67607032982621	8.83984734375575
H	36.66755425751690	-24.30636995912092	10.89998735034617
H	35.39808214062787	-25.33248890785167	11.56958320027559
H	39.56424720416067	-29.15220512627907	9.17527793950796
H	39.13201801854645	-27.50051550705404	9.63616760001702
H	38.10077144111732	-28.84912026786159	10.11895480433729
H	38.83984344015759	-30.82149137845204	6.06969889030709
H	39.84073880900275	-29.45597110224110	5.57197653006683
H	39.93286630025374	-30.06008674422458	7.23126557827354
H	35.16596421730542	-23.58222887882110	11.48992435252711
H	34.24848745950573	-31.29813216668779	3.76583597912280
H	33.87120528433325	-32.87961090698344	4.48825378003014
H	32.71622121070133	-31.53594865003866	4.62532031930012
H	33.91508478946466	-31.80994191582402	6.77505885279994
H	35.48264931672026	-31.64173842780693	5.94629479532442
H	31.84756906540448	-26.40751078523378	7.15521142500815
H	31.38539882348483	-28.07980911629459	7.55270084025532
H	32.58813193086417	-27.21998819656223	8.51935571208672
H	32.30643254256894	-26.91061663720022	1.98243637004948
H	36.77820284956098	-26.61080866222851	9.80124914847535
H	37.68576069951541	-29.51229241717562	4.20746500100673
H	32.33742293015941	-22.98806978516798	7.01139001675002
O	35.88950727556607	-25.34992134702935	5.11759854719915
H	35.59678232447703	-25.12502377156048	4.22146032745619

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B3LYP Scan/Hydroxide IPC Model/Triplet/30 degrees Constrained Optimization

C	30.55850110678417	-24.83377084875031	2.37032174109620
C	35.60116845349818	-24.42682101517097	10.94082423207157
C	39.23120152583096	-29.87401751179742	6.40923485505365
C	33.83350140864488	-28.73763565553751	0.64314195418648
N	33.16464230597833	-25.56289683765769	4.97182475818316
N	34.58886861342318	-25.47545877266773	7.48452429317300
N	34.85115782331320	-27.65971877621990	4.09084482142800
C	32.89519065711516	-26.81377053594730	2.89053049646648
C	32.88963212926589	-23.88042523161149	6.73264174805680
C	36.29183240904143	-26.59305985052082	8.83179549956216
C	36.92894212047712	-28.84525638153770	4.61220492422417
C	30.63578300687167	-22.79115578460297	4.90269617023595
C	33.38683504397317	-22.53607010536287	9.48287926365925
C	38.72434935204740	-28.46341847924152	9.29777448631609
C	36.63817818542618	-29.97198709458526	1.73727551226045
C	32.52546848937807	-25.81948333635774	3.79258335998942
C	33.81837673706349	-24.36312436449919	7.65194281425874
C	36.76366896338615	-27.47375556461070	7.86329568506159
C	35.87633422497191	-28.50044728548709	3.76899725185392
C	31.46581436392220	-24.84749981747740	3.56552907110842
C	34.05722305816483	-23.77426810019758	8.96444706816433
C	37.93490948151668	-28.32736263311627	8.02919223962122
C	35.69015680068319	-29.03420629645182	2.42653348867675
C	31.50053181217755	-23.98655692662482	4.63027489941680
C	34.98424981222637	-24.57095900769023	9.58074330827231
C	38.14739645695909	-28.91985465968995	6.81540371781680
C	34.51163846803423	-28.51143204275548	1.96226209088897
C	32.56600118551846	-24.45732866313043	5.50577189423729
C	35.31458089270335	-25.62240528718098	8.62741400289340
C	37.08598482860747	-28.44317722810716	5.93469088425457
C	34.01303178527589	-27.63586247658903	3.01318544232394
N	36.26626597651826	-27.58388613735463	6.60030458904822

Fe	34.68861107650711	-26.61032120592574	5.80866516284095
C	34.35473288238175	-31.38239076161088	5.98548774456092
C	33.86560203611579	-31.78434686092335	4.59787981846648
C	32.23021511681296	-27.37898952456218	7.51894783576922
C	33.31760089774716	-27.90491788768600	6.61267535644714
C	33.21312297035006	-29.33890572846368	6.44773115920709
O	32.17688862549500	-30.00943805759506	6.48610821177170
O	34.41149289711046	-29.96967711402485	6.16486216933714
H	29.90994957965547	-22.62580247968334	4.09872268463968
H	31.22976634085014	-21.87199175065376	5.00243174946117
H	30.06798288395635	-22.90456936211157	5.83675200140546
H	31.12035970061160	-24.73072424359008	1.43129392219079
H	29.97568420234294	-25.76206040784166	2.29108602467577
H	29.84520285554185	-24.00350266790925	2.41595494174980
H	33.66957083395114	-27.79605231585768	0.10084707289085
H	34.42677334785537	-29.38961397541638	-0.00757611309593
H	32.84872960570694	-29.20913164761917	0.76738524342691
H	36.32121610047702	-30.17911351406655	0.70928383302089
H	37.65461889267146	-29.55756769289313	1.69079174727657
H	36.71164920723404	-30.93755616926587	2.25684452572669
H	33.74289018836561	-22.27651266910922	10.48605808706460
H	32.29607263826770	-22.65696734098572	9.54413801221090
H	33.57463491067215	-21.66999752226547	8.83310083691557
H	36.68956375613215	-24.28607677060541	10.88136433877581
H	35.43003064656658	-25.31589642379922	11.56374816794876
H	39.56391103901234	-29.15649610087230	9.17514192040109
H	39.13957003276665	-27.50043157186877	9.62718426649038
H	38.10600311057240	-28.84223680290827	10.12382800040980
H	38.82289639478888	-30.83784819233444	6.07478055376482
H	39.83026606285019	-29.47678392976840	5.57776890678974
H	39.91857926593350	-30.08109880095147	7.23711158722578
H	35.18915171196610	-23.56699729253589	11.48039744516624
H	34.46849577766749	-31.30455488747260	3.82337014235975
H	33.92926292995615	-32.87243670827073	4.46864225928374
H	32.82767985028821	-31.47682164056229	4.46747928101771
H	33.71144718482194	-31.82462844615394	6.75226605613045
H	35.38274189006559	-31.72107738450055	6.14646610692877
H	31.84229586237509	-26.41030978541514	7.19522512898069
H	31.39448335870780	-28.08248336259819	7.59722423276629
H	32.62698165132292	-27.22270671338866	8.53393156134793
H	32.30988460980007	-26.90260171033637	1.98023625872549
H	36.78892501458503	-26.60275817053378	9.79747538676225
H	37.67334781492262	-29.52930042397358	4.21478465144066
H	32.33388947412603	-22.99154996224425	7.01701369561938
O	35.89208935234042	-25.35700940240173	5.11762344947816
H	35.59073394295333	-25.12069848791102	4.22731290836588

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B3LYP Scan/Hydroxide IPC Model/Triplet/40 degrees Constrained Optimization

C	30.57104827552662	-24.74818835115795	2.34592359797257
C	35.57395007735267	-24.48343311899310	10.94401110583290
C	39.18390753150909	-29.90779799213610	6.35719130381694
C	33.78588443909487	-28.69426952939416	0.60795126262087
N	33.15650912974741	-25.53061876147530	4.95271306358012
N	34.58002793427850	-25.47420775087764	7.46519533621746
N	34.82268164378829	-27.64128702578792	4.05754688012495
C	32.87930955073379	-26.76197432451523	2.86039580898519
C	32.88668860949046	-23.86504982174393	6.73044192569465
C	36.27662078060310	-26.61356260700715	8.80243340281244
C	36.88903014720628	-28.84984879437429	4.57006135328968
C	30.65363306803857	-22.73473650300227	4.90163710908677
C	33.36830650129264	-22.56807084988003	9.50626788523175
C	38.69315819611673	-28.50786018050161	9.25460372260077
C	36.57149040745686	-29.97443330766532	1.69543480079873
C	32.51967956540523	-25.76954935104144	3.76863478709571
C	33.80968646960497	-24.36399561163221	7.64696251470343
C	36.74639498333161	-27.48516753348485	7.82478857947560
C	35.83561883466265	-28.49555729945743	3.73140932155329

C	31.47115918319275	-24.78425306830989	3.54605858828922
C	34.04237726801085	-23.79649974507465	8.96981751732074
C	37.90785367219042	-28.35285378624581	7.98573194995188
C	35.63940813192109	-29.02353217157383	2.38808303092672
C	31.50841453400791	-23.93526199722942	4.62016440450386
C	34.96625285993093	-24.60344707649864	9.57752677935311
C	38.11363619618189	-28.94077090934760	6.76863489771322
C	34.46930953473708	-28.48076887112039	1.92630857970050
C	32.56527424575715	-24.42519365157786	5.49547129572610
C	35.30091397566959	-25.63928868553842	8.60897580528381
C	37.05795609097040	-28.44651581405274	5.89082506822158
C	33.98441704193236	-27.60132960504325	2.98022816712639
N	36.25016895041306	-27.57962383547541	6.56048002149091
Fe	34.67645474848936	-26.59401518443021	5.77952817492880
C	34.41674898993598	-31.39722978378293	6.24959406163996
C	34.19437115933790	-31.86030140822860	4.81385231938671
C	32.19972057800601	-27.37744006526834	7.46539641678804
C	33.30289665597884	-27.89754126510617	6.57363187133742
C	33.22547676588871	-29.33704574669037	6.43498757684622
O	32.19464381477690	-30.00128488815769	6.30928503303141
O	34.45191897025757	-29.97643681219243	6.37706499042437
H	29.93090473096708	-22.55557238782289	4.09781747986250
H	31.25539033923366	-21.82172824054356	5.01106964401964
H	30.08285583265960	-22.85177846478333	5.83341654317960
H	31.13952223718576	-24.63963139252099	1.41149637311643
H	29.97993643742010	-25.66988343996635	2.25251154632876
H	29.86539558839893	-23.91169418563325	2.39688803687809
H	33.62999284713369	-27.74865742919183	0.07029665275423
H	34.37124280138355	-29.34893562840900	-0.04718022604779
H	32.79664149061389	-29.15636704854900	0.73243809928436
H	36.25072642749383	-30.17246348469000	0.66680832732197
H	37.59464607339519	-29.57670949323940	1.64975794596742
H	36.62967792972479	-30.94351604974413	2.21069727804872
H	33.71964566811805	-22.32564693170140	10.51536722292129
H	32.27740878927844	-22.69108998849426	9.56048361244252
H	33.55802310713723	-21.69070550705121	8.87237310112568
H	36.66285294946596	-24.34274473656016	10.89466135511596
H	35.39777805296770	-25.38326322920195	11.54986390896174
H	39.52982644630928	-29.20337193531659	9.12602147323719
H	39.11181618500990	-27.55090322598851	9.59683386125621
H	38.07066764126466	-28.89378039690165	10.07429870859060
H	38.76192598043894	-30.86588702319657	6.02316792308854
H	39.78468545098197	-29.51722485219647	5.52383439574671
H	39.87181402801885	-30.12470588875575	7.18211811704724
H	35.15878273900250	-23.63287998385193	11.49575290646021
H	34.93956901571464	-31.41876322889159	4.14865056948635
H	34.26795070085304	-32.95342479301892	4.74759183086822
H	33.20421183414562	-31.55677510608140	4.47297654507311
H	33.63645553040046	-31.80420062358095	6.89945764567525
H	35.39262109628228	-31.72951413700798	6.61645340058588
H	31.82499617095580	-26.40017117200844	7.15309572240440
H	31.35493671041187	-28.07479574112167	7.50831296060193
H	32.57218231482022	-27.24696502326859	8.49368326130046
H	32.29490100703974	-26.83689132791124	1.94826421206861
H	36.77049515992045	-26.63773519047000	9.76950791107245
H	37.62273786981942	-29.54409470661599	4.17030885640239
H	32.33373495132393	-22.97752168754380	7.02418584392753
O	35.88496362426628	-25.34601482056571	5.09030628005936
H	35.58210073161511	-25.10377499253092	4.20209526028148

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B3LYP Scan/Hydroxide IPC Model/Triplet/50 degrees Constrained Optimization

C	30.57839283223531	-24.68552439799040	2.33549013082573
C	35.57099415255139	-24.51491487635929	10.94230231497917
C	39.15259421596861	-29.93047910077708	6.32123842162006
C	33.74480593188748	-28.66720114903443	0.58896085628989
N	33.15308389467223	-25.50392077065016	4.94189107898432
N	34.57122830931466	-25.47664734125718	7.45670738857074

N	34.80415570832373	-27.62373769169010	4.03452245779994
C	32.87122716113153	-26.71823696186921	2.84008105616315
C	32.88234038044856	-23.85638146493329	6.73602735953865
C	36.26988958356991	-26.62688737481465	8.78245491665864
C	36.85554269842633	-28.85853411982353	4.54390463634866
C	30.65939429935408	-22.69925471068850	4.91283765701504
C	33.36396285077691	-22.58716992775727	9.52448762611978
C	38.68117151663910	-28.52937263019674	9.22119064137275
C	36.50620523968748	-29.99586346714301	1.67775047048600
C	32.51827821782121	-25.72879484515644	3.75408251425853
C	33.80231413766558	-24.36701800807476	7.64905673293583
C	36.73477865856037	-27.49481901297139	7.79962452170952
C	35.80331118524175	-28.49382506968276	3.70763441037150
C	31.47478623142194	-24.73672148143777	3.53775727943417
C	34.03659967350075	-23.81127283569332	8.97641986830770
C	37.89216256450770	-28.36890400031468	7.95532229507839
C	35.59611303350677	-29.02140336911163	2.36598325792013
C	31.51133571837875	-23.89926667219481	4.62079561476123
C	34.96129704416853	-24.62352459233956	9.57574649548333
C	38.09008905154352	-28.95693043282815	6.73713104109189
C	34.43474131827941	-28.46010446931725	1.90490494891893
C	32.56361883875098	-24.40217306040918	5.49411040204536
C	35.29375336765536	-25.65141398926029	8.59822034967887
C	37.03401862417179	-28.45530517488395	5.86374332214434
C	33.96500604724991	-27.57194053616434	2.95824988836497
N	36.23479634067096	-27.58317802151977	6.53640399570963
Fe	34.66835156216976	-26.58158787510774	5.76119035719217
C	34.38491337872094	-31.41914541136775	6.42766025678741
C	34.51917046527048	-31.88981083774323	4.98408110847353
C	32.16397820212048	-27.39112341994418	7.40908030383313
C	33.28579036843374	-27.89611652986752	6.53154144790421
C	33.21469683783651	-29.33597179567559	6.36839641666822
O	32.21787510118208	-29.97811074523636	6.04205951654103
O	34.41844293308549	-29.99633888173912	6.55265354535454
H	29.93684317053038	-22.51154017267060	4.11081248009001
H	31.26307469397667	-21.78844223224599	5.03005616420421
H	30.08856652036637	-22.82319952034076	5.84368045462792
H	31.14993532391442	-24.56864327711006	1.40393930230379
H	29.98529738601534	-25.60471098954140	2.23075382893873
H	29.87476845313054	-23.84775514648483	2.39320525138760
H	33.59513201829445	-27.72004261844592	0.05228180869887
H	34.32239398532316	-29.32647201975239	-0.06842277784285
H	32.75210210874886	-29.12078533900825	0.71702853985248
H	36.19100781384094	-30.17835856356076	0.64447775729932
H	37.54169886964063	-29.63015296261212	1.64506951692034
H	36.52761693360491	-30.96877441597999	2.18867367985640
H	33.71622259250585	-22.35437190695825	10.53552513767395
H	32.27297981155274	-22.70962786860009	9.57825521136034
H	33.55408200697018	-21.70415369806562	8.89859402917961
H	36.66000445096139	-24.37519095748328	10.89246663989770
H	35.39465933134298	-25.41922877726515	11.54139751335263
H	39.51649269689699	-29.22559692639714	9.08776537607551
H	39.10218638999047	-27.57412535439726	9.56528466793947
H	38.06068149824384	-28.91712750241602	10.04154058839701
H	38.72427774414032	-30.89039689100391	6.00064538749272
H	39.74456090513407	-29.54865725977934	5.47766140888486
H	39.84971699731130	-30.14219844457220	7.13980002322972
H	35.15772726373912	-23.66811161683320	11.50122538285515
H	35.43064831512332	-31.49092653784730	4.53376317015448
H	34.55718199079497	-32.98583694116614	4.94041657223928
H	33.66584790460121	-31.54683915906629	4.39783338294918
H	33.45697776112135	-31.80108518140056	6.86194996214558
H	35.22970536375295	-31.76951435728764	7.02859216194658
H	31.81126946341087	-26.39796112364129	7.12265989594257
H	31.30540841846036	-28.07480640049352	7.39873667032865
H	32.50282864587247	-27.30513984413327	8.45437558766577
C	32.28687988711706	-26.78307865442833	1.92715204676286
H	36.76610104653945	-26.65733525492401	9.74815800808939

H	37.58247428221146	-29.55828090567457	4.14130934340014
H	32.33108395145165	-22.97048973427406	7.03773582968450
O	35.88428631017170	-25.33822613952736	5.07944758604252
H	35.57908602029354	-25.08391483095768	4.19539040423201

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B3LYP Scan/Hydroxide IPC Model/Triplet/60 degrees Constrained Optimization

C	30.56640994593721	-24.67212660471937	2.34208096990023
C	35.57933374194700	-24.51856881599523	10.93606243897749
C	39.12678215934521	-29.95659998458844	6.31068189268939
C	33.72479273336908	-28.65810275443166	0.58245710976901
N	33.15993419128429	-25.48246522431388	4.93216774743121
N	34.57784827148977	-25.46628829524240	7.44678376342234
N	34.80931284007237	-27.59933112538596	4.01516051282221
C	32.87448171984954	-26.69100201873179	2.82719737809942
C	32.88126431897557	-23.84891816414455	6.73788031152272
C	36.27729015419018	-26.62127878122429	8.76766411013013
C	36.84632586667315	-28.85591082722598	4.52826434503145
C	30.64038206786397	-22.70081835843150	4.93101754298096
C	33.36307465096948	-22.59173971332124	9.53171018639903
C	38.67050965165318	-28.54521720262192	9.20765266005733
C	36.47720420804770	-30.00688516530886	1.67007821333666
C	32.52189720669951	-25.70576768649708	3.74565773235646
C	33.80536248819193	-24.36020048276572	7.64632138556895
C	36.73671022826284	-27.49081363722870	7.78394589514756
C	35.79855535317133	-28.48140020684291	3.69043573160236
C	31.46992292769744	-24.72081657543741	3.53908108531156
C	34.03968737988764	-23.81020499583395	8.97604569256471
C	37.88497659680419	-28.37634159372933	7.94068836811519
C	35.58173261942123	-29.01540592754635	2.35285725052709
C	31.50326206039854	-23.88999554212745	4.62727375292553
C	34.96831344357386	-24.62205954277315	9.56968929619394
C	38.07709904715423	-28.96807791710992	6.72340679902447
C	34.42442178796752	-28.44541685381586	1.89230090975826
C	32.56306286356143	-24.38944447998783	5.49344302417711
C	35.30189998952250	-25.64450305740646	8.58688705125604
C	37.02769060439736	-28.45499071101356	5.84863057052034
C	33.96601964754442	-27.54758440987178	2.94228553164163
N	36.23705530618138	-27.57395074866078	6.51996072232634
Fe	34.67801973623192	-26.56028102450529	5.74351152631152
C	34.32576638359281	-31.43123054277074	6.50467390926286
C	34.67057426019411	-31.89721579632087	5.09504422340214
C	32.17405080305900	-27.41001290868755	7.39465369729917
C	33.29214989609156	-27.88331339333324	6.49567127782279
C	33.22686628489068	-29.31906218075062	6.27692102929399
O	32.29158472819406	-29.92851850704206	5.76829143484727
O	34.36899323990109	-30.00891396358936	6.65230644032919
H	29.91563035300080	-22.51250858311419	4.13110221900268
H	31.23540134935156	-21.78541006603106	5.05643631002747
H	30.07108278008327	-22.83872470819411	5.86088510960918
H	31.13201243357780	-24.55289702216789	1.40725282126323
H	29.97611687405580	-25.59350231276592	2.24054463202359
H	29.86003522851126	-23.83698307795493	2.40428152430452
H	33.56837279394465	-27.71297026944389	0.04424732972251
H	34.29888947483074	-29.31791468588791	-0.07746145081259
H	32.73444302647185	-29.11390461014389	0.72032215319113
H	36.15578401659707	-30.19519067377611	0.63976289295096
H	37.51721362990637	-29.65481721980947	1.63010915382042
H	36.48768387984440	-30.97463065717645	2.19081124254895
H	33.71788442439843	-22.36153061674321	10.54246306342358
H	32.27286588991061	-22.71970932182763	9.58894972568330
H	33.54654647247714	-21.70513599543025	8.90893264225085
H	36.66812501240495	-24.37735206303171	10.88573596380627
H	35.40478313211747	-25.42568140018980	11.53149224857283
H	39.50343179290243	-29.24415949511908	9.07338661530119
H	39.09455268830801	-27.59303201946488	9.55642278692069
H	38.04675313260924	-28.93374371701605	10.02519274698126
H	38.68622749713077	-30.91404925686242	5.99910351813291

H	39.72026389785752	-29.58833469355844	5.46220846528353
H	39.82429162366358	-30.17041611020259	7.12841173603720
H	35.16562096664711	-23.67469489884607	11.49911613751236
H	35.64863272602169	-31.51620415304395	4.79315943482117
H	34.69299867701265	-32.99364885073576	5.05056872474269
H	33.92495251643614	-31.53414285634539	4.38697219133351
H	33.33414187639217	-31.79545004851941	6.78721547970544
H	35.06062414337599	-31.80421055896489	7.22475213477861
H	31.83304227275077	-26.40066234924341	7.15357166064830
H	31.30356012001970	-28.07920521529848	7.34788078115178
H	32.50507958259713	-27.37746110002030	8.44628213706953
H	32.28609149457168	-26.75572180851909	1.91689644091648
H	36.77387698275695	-26.65518511552044	9.73305521567446
H	37.56607978794854	-29.56364420145677	4.12680011644566
H	32.32529053574675	-22.96819759787036	7.04604779649651
O	35.89604455079848	-25.31767379518549	5.06739179211190
H	35.59196696270814	-25.06054973318322	4.18378788438990

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B3LYP Scan/Hydroxide IPC Model/Triplet/70 degrees Constrained Optimization

C	30.64428757671753	-24.52956748570809	2.27001023501392
C	35.44353779507960	-24.67903851314142	10.98426140073419
C	39.09761507104013	-29.97205831005299	6.26192942419577
C	33.77444516028681	-28.52706692865217	0.48933157866637
N	33.16666059074695	-25.43941489159442	4.89782558658892
N	34.53877446473351	-25.49551498292153	7.43580675079333
N	34.82254082801990	-27.54340430723728	3.95528419760745
C	32.92387899725061	-26.58179593565206	2.75079340606466
C	32.84220072862519	-23.86806186849932	6.75081166230070
C	36.22202991554401	-26.68157198055118	8.75033562317181
C	36.82761556982393	-28.84667674992581	4.47919887723017
C	30.64997656431155	-22.65479789231383	4.93022265445831
C	33.23742267110708	-22.72351320075778	9.60600575937508
C	38.61307645298871	-28.60933274114247	9.17768608454075
C	36.46941347635067	-29.96319844691179	1.60677726493788
C	32.55803839094009	-25.62026523158478	3.68865471783239
C	33.74865913425871	-24.40704634603548	7.66103717548650
C	36.69959966967237	-27.52326278637124	7.75125175286857
C	35.79681052810090	-28.44348122246284	3.63375066025249
C	31.51462295486830	-24.62466341938461	3.48851007111820
C	33.94531431273866	-23.90780255193014	9.01665055410716
C	37.84267369165666	-28.41541180495406	7.90513824347542
C	35.58929402371572	-28.95569456074532	2.28621491401807
C	31.52004768540565	-23.83337809427633	4.60610653629271
C	34.87080218875742	-24.73113910048067	9.59871580271141
C	38.04463578676247	-28.98930568958108	6.68076805554672
C	34.45577201028902	-28.34986733135213	1.81373685348412
C	32.55674239763999	-24.36478501450492	5.48073538622336
C	35.23985000268514	-25.70967884026065	8.58457014157628
C	37.00576162967401	-28.45852121687827	5.80414719778479
C	33.99910660309548	-27.45814037101201	2.86967385406362
N	36.21583678692483	-27.57995586219528	6.47967050977500
Fe	34.67235345928385	-26.53962811574337	5.70466877270535
C	34.29886725602213	-31.43573492171580	6.77709642269629
C	35.01238309496785	-31.95321061968952	5.53432863235926
C	32.08525867766588	-27.48178331620327	7.20737460084854
C	33.29346946416078	-27.89869002106223	6.40346174163474
C	33.30805470711509	-29.33976235124085	6.18008119236114
O	32.54840509394469	-29.97139894429259	5.45980402152744
O	34.30623204666004	-30.00727472848598	6.87646978745920
H	29.93872515731044	-22.44351411463191	4.12392635005751
H	31.24062752096001	-21.74249433117584	5.09364760649975
H	30.06503189744893	-22.82183775571749	5.84548536326835
H	31.23523463443942	-24.37183600575671	1.35675106172449
H	30.05947854685227	-25.44701172816835	2.11508694049975
H	29.93434158535389	-23.69862235201419	2.34629909592753
H	33.65318935388344	-27.57128054614268	-0.03923889576147
H	34.34246992706442	-29.19366782157789	-0.16896411230795

H	32.76997477859759	-28.95764904071358	0.60418452300250
H	36.16773558944337	-30.12259316174140	0.56563449230115
H	37.52076314407124	-29.64436264531848	1.59804626343246
H	36.43638619319704	-30.93971760607865	2.10997351029858
H	33.56479339192993	-22.53065369523475	10.63369779984222
H	32.14829566836077	-22.86950610957272	9.63154465860335
H	33.42160894861649	-21.80875651333267	9.02554988834156
H	36.53167318924871	-24.52492198670519	10.97020586317195
H	35.26299986613212	-25.61264553338221	11.53529940837795
H	39.44700157418387	-29.30644491166503	9.04011133370615
H	39.03328856538494	-27.66446719005328	9.54994294754020
H	37.97896533064071	-29.01312469145119	9.97974668019561
H	38.66178310629649	-30.92577499397141	5.93258607712232
H	39.69726906107982	-29.59078490933524	5.42367592857568
H	39.78854381107109	-30.19743937689158	7.08207980725537
H	35.00531910833886	-23.86416768181292	11.57103047965393
H	36.04102574830806	-31.58767100077848	5.49951921480542
H	35.03075977539052	-33.05050404869417	5.53504310779770
H	34.49509000197452	-31.61348708307334	4.63646247692404
H	33.26531990013770	-31.79282760466585	6.79130832181920
H	34.80596969497353	-31.77816726962470	7.68443685506166
H	31.84513248346684	-26.42425876699173	7.09199183357293
H	31.19149739690580	-28.06002033573269	6.92465876869315
H	32.23978248086317	-27.65263498198486	8.28824321514611
H	32.35525945858615	-26.61607736476476	1.82632894623760
H	36.70209177693228	-26.74205540127016	9.72273812734855
H	37.53697238397265	-29.56550710371086	4.07925105434059
H	32.27386029808165	-23.00219482765267	7.07792821503697
O	35.89977174346212	-25.28737990724900	5.07002627409918
H	35.61409342540635	-25.01896323085579	4.18364819689991

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B3LYP Scan/Hydroxide IPC Model/Triplet/80 degrees Constrained Optimization

C	30.65408664145746	-24.40215979107649	2.22218366000878
C	35.44523290672628	-24.78468546169188	10.93964955951141
C	39.05818685193541	-30.00045239792519	6.08031340722001
C	33.71699217548470	-28.40235433788252	0.36792199600587
N	33.11345343161142	-25.43805990381110	4.86171060460041
N	34.53445889220662	-25.51952558361746	7.37328799385467
N	34.76854871118881	-27.52218574820600	3.86120557479049
C	32.88937542614649	-26.50659757717944	2.67649927132172
C	32.80079239768084	-23.90518874764831	6.74660594471627
C	36.23769592531075	-26.72085737328512	8.65219686842785
C	36.75557892637319	-28.86195092089930	4.35065856359847
C	30.64753645932479	-22.61002865135014	4.93788194396766
C	33.19368299836767	-22.83501808466194	9.62916790736236
C	38.63453753146027	-28.65532834846850	9.01612016192472
C	36.37471867966410	-29.92088917900743	1.46167421581171
C	32.52589058482223	-25.56949685573852	3.63909417942484
C	33.71973573320701	-24.45558102213601	7.63754576570520
C	36.69766598678201	-27.55484150243125	7.63722220040727
C	35.72662978729231	-28.42848573059041	3.51984301422982
C	31.49760580913424	-24.55352045682503	3.45355768857236
C	33.91882185799269	-23.98987077895747	9.00306701883123
C	37.83720748776324	-28.45191360612694	7.76136319423867
C	35.51336861397356	-28.91014898464910	2.15911724144007
C	31.49797986081633	-23.79706824474512	4.59381807365213
C	34.86611051726211	-24.81001086241096	9.55592895628827
C	38.01260289070813	-29.02159274008540	6.52794909079774
C	34.39653940045265	-28.27179726045469	1.69821692800108
C	32.51722748911167	-24.36938958265765	5.46451862647747
C	35.24371836381281	-25.75590282746402	8.51636490553053
C	36.96185904500623	-28.48282271477235	5.67511938476967
C	33.95395587513261	-27.39563631361324	2.77686256216593
N	36.19332182917534	-27.59552958097230	6.36952137221076
Fe	34.63551452963768	-26.54078546405307	5.62003203777093
C	34.18663289865850	-31.39175773396218	7.23511524684868
C	35.42016579385403	-31.88486188913923	6.49106554071813

C	31.91696866618147	-27.58270974140125	6.84042186057272
C	33.29430271582773	-27.92755677171842	6.33089069715398
C	33.45142558790285	-29.37106197765998	6.16350071743883
O	33.06200215360813	-30.06202377882119	5.23855975336128
O	34.09330612491649	-29.96266348168097	7.24712316423639
H	29.92995918543222	-22.38329786482810	4.14145652608797
H	31.25246396216284	-21.70674432862570	5.09990277937352
H	30.07143821479105	-22.77568851350448	5.85895292653499
H	31.25957810539757	-24.14931992000256	1.34007917592636
H	30.11416061894964	-25.32845052071240	1.98197614586235
H	29.90655823338866	-23.61007303334823	2.34177278298751
H	33.61221692072271	-27.43031180554145	-0.13360675929640
H	34.27778681056897	-29.05850633262046	-0.30690350714473
H	32.70582532070160	-28.82150618963279	0.46703669763791
H	36.07493154385174	-30.05035950628020	0.41578174051730
H	37.43297773063687	-29.62567952366582	1.46455056026474
H	36.31686789321405	-30.90769581835959	1.94231721399570
H	33.53360652822596	-22.65536593694817	10.65516157090946
H	32.10882893252759	-23.00683751927246	9.66905001670959
H	33.34656892295360	-21.90435134110591	9.06503197459659
H	36.53539316237450	-24.64572159239528	10.92353950344181
H	35.25405288148285	-25.72313788530210	11.47883444061094
H	39.45644194046903	-29.36265626181585	8.85984815029664
H	39.07486978633777	-27.71596836805508	9.37938433765359
H	38.01354495507184	-29.05133486281934	9.83183354792842
H	38.61613349657203	-30.95530199799505	5.76371248948507
H	39.63144165260650	-29.61575454738025	5.22554634839669
H	39.77319590337805	-30.22235661959474	6.88058955490612
H	35.02091141705628	-23.97181639208637	11.53926167854451
H	36.32366796457809	-31.43621296467216	6.91091829440168
H	35.50187987198732	-32.97676476224850	6.56329099702393
H	35.35811067549894	-31.60745538839054	5.43786652026299
H	33.28067089134647	-31.81057740824924	6.78917389860869
H	34.23002380331226	-31.67883950112935	8.29067652922293
H	31.80688717562166	-26.51900761821279	7.05354300666194
H	31.13254191298697	-27.85143249373414	6.11037321444453
H	31.67048837590619	-28.13036720314120	7.76735392296508
H	32.32984050906824	-26.50489588727265	1.74577751743545
H	36.72926203634392	-26.79569759474089	9.61769271810859
H	37.44787308180565	-29.58936673850377	3.93692542437286
H	32.22945873014012	-23.05057181712757	7.09730319313544
O	35.83516235391793	-25.27577633275584	4.96002076164680
H	36.44313491864116	-25.04240592515171	5.67786299451522

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B3LYP Scan/Hydroxide IPC Model/Triplet/90 degrees Constrained Optimization

C	30.62435963883825	-24.43051387377238	2.23619495212079
C	35.48060728187567	-24.76390262936495	10.92096496621517
C	39.04547355640504	-30.02503753344260	6.07472592887097
C	33.74934579823225	-28.36482057732994	0.34284762192643
N	33.11437579236149	-25.43872822943386	4.85719087452967
N	34.54402846563195	-25.51491615086829	7.36473624263400
N	34.79039097267132	-27.50053879641552	3.84293111625969
C	32.90037009526610	-26.49648631309095	2.66594468683169
C	32.79076715245442	-23.91728569852807	6.74982987999013
C	36.26014612949194	-26.70686533710237	8.63583020653798
C	36.77349247802788	-28.84612222036994	4.33254265222968
C	30.60158611888536	-22.65353381323199	4.96200960497144
C	33.20204911160117	-22.83519536453126	9.62613413144070
C	38.64474726273046	-28.65588161796309	9.00267198399553
C	36.41132360921377	-29.87807488095790	1.43310705685649
C	32.52406682478527	-25.57226781254030	3.63615598565914
C	33.72335101369993	-24.45636106746701	7.63344324288802
C	36.71509624226501	-27.54463582843763	7.62185539299785
C	35.75135788076989	-28.40226228332602	3.49904524995341
C	31.47803050008327	-24.57270399828938	3.46167834385684
C	33.93021253380795	-23.98612467564325	8.99625082906363
C	37.84777191240530	-28.45034341925470	7.74788567031448

C	35.54406370723389	-28.87527269155668	2.13446291246804
C	31.47137707655888	-23.82295677406163	4.60645192826205
C	34.88833826423016	-24.79787086379410	9.54293245651252
C	38.017110885280217	-29.02593066364173	6.51642848495513
C	34.42541284347392	-28.23934371258258	1.67534616227035
C	32.50457340551647	-24.38287950438233	5.46881401448901
C	35.26335304741325	-25.74409039487113	8.50284087155462
C	36.97371924189365	-28.47739154104359	5.66088604730317
C	33.97599477611831	-27.37290553518146	2.75900296517757
N	36.20953752288040	-27.58517091287666	6.35421757729705
Fe	34.64805830086807	-26.53033078780300	5.60581189885192
C	34.03398900155290	-31.42944701725736	7.21437742710646
C	35.36647048252794	-31.90451432131327	6.64938519190452
C	31.96177607387043	-27.59215513825660	6.87290819179748
C	33.32141533835637	-27.92663612487205	6.31506510041064
C	33.48460664780342	-29.36390873632208	6.11084387325273
O	33.22652697706140	-30.02011447300861	5.11823404245958
O	33.94640967703401	-30.00113338049229	7.26186616710404
H	29.87972829880695	-22.43159538697540	4.16809427716176
H	31.19129553478895	-21.74169538788059	5.13188915350053
H	30.02887886693591	-22.83710812633547	5.88185469885070
H	31.22080766165383	-24.17058542744106	1.35003783742822
H	30.09341057973214	-25.36290319476245	1.99939113122372
H	29.86868026422943	-23.64705622152631	2.36121476049526
H	33.64787643536378	-27.39124987011624	-0.15652064597965
H	34.31069932604347	-29.02045861957946	-0.33200869448616
H	32.73715462257375	-28.78240588625171	0.43803196709395
H	36.11427855090410	-30.00317967310384	0.38590702797306
H	37.46822126639922	-29.57800515375180	1.43994509190618
H	36.35675406769442	-30.86764981728633	1.90833125550599
H	33.54544140485120	-22.65459672054685	10.65080678453399
H	32.11824653261757	-23.01245885756478	9.67046981342251
H	33.34790163937533	-21.90338307495535	9.06201410245440
H	36.56685089729376	-24.59771446104925	10.89464154055629
H	35.31834794550488	-25.70918508896868	11.45753381309856
H	39.46328818696625	-29.36716886804236	8.84675643132040
H	39.08988531795553	-27.71786956626753	9.36360566933799
H	38.02302519620355	-29.04740114213158	9.81997839319954
H	38.58560205779797	-30.97626655803425	5.77269209690993
H	39.61993345208452	-29.66022411335733	5.21209261528805
H	39.76144725505171	-30.24844371586704	6.87372089730638
H	35.04231926529320	-23.96446347667090	11.52852111326280
H	36.19872999740653	-31.47928031622791	7.21624031603735
H	35.43540958974659	-32.99886428392990	6.69184607644034
H	35.46507959521967	-31.58864376842842	5.60990744972258
H	33.20695756023259	-31.82515373174044	6.61900360233624
H	33.91412208057734	-31.75447241760326	8.25297480977886
H	31.88343830373691	-26.54708525260764	7.17586745892088
H	31.16089669176555	-27.77470283400974	6.13349393908370
H	31.71273306574663	-28.21066642088868	7.75242789298839
H	32.33939688231093	-26.49624192408437	1.73605001296038
H	36.75584229587510	-26.77900819519587	9.59944065973397
H	37.46497704683020	-29.57352199940689	3.91740039342659
H	32.21169021962279	-23.06989609894113	7.10535131792363
O	35.84218568351623	-25.25518057697911	4.95207991707874
H	36.44697873059197	-25.01947940381198	5.67184887188338

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B3LYP Scan/Hydroxide IPC Model/Triplet/100 degrees Constrained Optimization

C	30.60760944413931	-24.45412288252835	2.23693855715809
C	35.49443077735863	-24.74540951845641	10.90567507052499
C	39.04174686165266	-30.03173866398496	6.07425779767397
C	33.77863110848730	-28.33896557300799	0.32438752163781
N	33.10839095606939	-25.44595284498774	4.85421402129805
N	34.54893369026428	-25.50780798450878	7.35407898791491
N	34.80217305802625	-27.48918799653508	3.83322627104473
C	32.90381853640861	-26.49823494559107	2.65921537384088
C	32.78212115068413	-23.92284430239510	6.74474794281691

C	36.26882066756366	-26.69534454789708	8.62578833311264
C	36.78957131234890	-28.82944799551424	4.32168743420395
C	30.57403579654022	-22.68042197476697	4.96433457404212
C	33.20560829208957	-22.82696715026231	9.61355709682891
C	38.64050648875112	-28.66040007540362	9.00094406660020
C	36.44889011515470	-29.83868176955792	1.41359296889761
C	32.51769340782749	-25.58253251611578	3.63339759804071
C	33.72480155431318	-24.45174508602792	7.62362596058222
C	36.72289955612188	-27.53604973343221	7.61386121499777
C	35.77028090886768	-28.38211202487869	3.48698185561160
C	31.46291673715704	-24.59196115965874	3.46183729569149
C	33.93546857911921	-23.97710123153161	8.98416581981243
C	37.85033723429075	-28.44781191993796	7.74308258116823
C	35.57096182107333	-28.84793535547418	2.11869354405592
C	31.45158465136790	-23.84366496742976	4.60758034344972
C	34.89817917219755	-24.78442103096029	9.52949426349354
C	38.02025890142854	-29.02396935512367	6.51195270416960
C	34.44854929333742	-28.21855820660269	1.66042189865013
C	32.49120082882300	-24.39531055025946	5.46736858646140
C	35.27243251964036	-25.73231895030146	8.49077997613220
C	36.98362149737966	-28.46833577138732	5.65291202030054
C	33.98888147804779	-27.36312207761414	2.74865092006798
N	36.22060839690197	-27.57394472513150	6.34478184921817
Fe	34.65184960463529	-26.52539921918741	5.59664594673476
C	33.92514385219763	-31.46623891837609	7.18540201546239
C	35.29093150957811	-31.93632600857484	6.69950486008620
C	32.03554380982533	-27.59829954537062	6.97985210640025
C	33.34653967802647	-27.93428811134037	6.31653138939294
C	33.50464467928787	-29.36566680759720	6.09011729208456
O	33.33266278516260	-29.99776825815454	5.06363975492841
O	33.84404626510645	-30.04039625282230	7.26717893703549
H	29.84513801750417	-22.46785952153987	4.17426615039073
H	31.15695052080508	-21.76280611416763	5.12664657632067
H	30.00880785611212	-22.86495561031970	5.88855902876035
H	31.20250388107572	-24.19203976312948	1.35038141742559
H	30.08034829880208	-25.38874582172063	2.00060744841852
H	29.84885991932330	-23.67364835785002	2.36197788912328
H	33.68388971861099	-27.36431054514830	-0.17441300872245
H	34.34056238433813	-28.99611121235518	-0.34853140386586
H	32.76423561102411	-28.75235802176759	0.41383478497883
H	36.15641986619553	-29.95919147949287	0.36455515453803
H	37.50320045226221	-29.52986869816815	1.42592803291447
H	36.40080118805179	-30.83170200545343	1.88224488613733
H	33.55115917150657	-22.64312725836201	10.63691891770658
H	32.12246629128361	-23.00734951284134	9.66128098622188
H	33.34710879282224	-21.89601778960358	9.04691558588184
H	36.58084530204794	-24.58133690658849	10.87558293415789
H	35.33195766340220	-25.68801807092595	11.44693875859776
H	39.46508423469240	-29.36426529502771	8.84325217553015
H	39.07654437863387	-27.72286023574823	9.37381790163591
H	38.01650209350447	-29.06430960160606	9.81052587046386
H	38.57510550313981	-30.98083146130515	5.77594310484774
H	39.61894996137821	-29.67472061478834	5.21018532645485
H	39.75604040390606	-30.25713776910709	6.87419175401689
H	35.05915845288658	-23.94258036223895	11.51090591422645
H	36.08584362673229	-31.52094312873972	7.32470928573498
H	35.35682283494744	-33.03124032727602	6.72933407391470
H	35.45469517743115	-31.60391967488969	5.67357705942474
H	33.13933484073068	-31.83953650943539	6.52285985560361
H	33.73113687309539	-31.82020187569283	8.20323338078345
H	32.00743999186282	-26.57291084905641	7.35210838499317
H	31.18810738863431	-27.70674618543492	6.27895049184708
H	31.82057954804273	-28.26716645248893	7.82929913679240
H	32.34357412470125	-26.49929525568002	1.72887904747536
H	36.76383883795641	-26.76619316458039	9.58983380638015
H	37.48303482364187	-29.55424323558727	3.90534433225821
H	32.19888789410761	-23.07874934536487	7.10126323542200
O	35.83785986016208	-25.24450944598868	4.94044398639010

H 36.44307121539186 -25.00730683884046 5.65932676819440

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B3LYP Scan/Hydroxide IPC Model/Triplet/110 degrees Constrained Optimization

C	30.58058779489853	-24.48731039591275	2.25588353393370
C	35.52677929438414	-24.72115003321051	10.89270594831609
C	39.06295029756737	-30.01550159173180	6.06442209956420
C	33.79220147804457	-28.33143343887842	0.32108861024158
N	33.11213221738044	-25.44750478248805	4.85520005344839
N	34.55901324646697	-25.50362659122731	7.35122576593684
N	34.82673991350749	-27.46619434838575	3.82245067061097
C	32.90983185558292	-26.49874263271997	2.65975035355528
C	32.78049113796791	-23.92896256226961	6.74844943725882
C	36.28921201975906	-26.68171230434794	8.61796071487231
C	36.81802864798989	-28.80172286108854	4.30816400354873
C	30.54369534991521	-22.71467632729400	4.98375735950636
C	33.22217324575469	-22.81688081499265	9.60805053335675
C	38.66178081709091	-28.64578391101420	8.99121073263495
C	36.47924940876701	-29.80842963630292	1.40110857004892
C	32.51601670806650	-25.59019767706748	3.63761435285948
C	33.73250623781495	-24.44929590803198	7.62209919647277
C	36.74318830672889	-27.52183911455280	7.60540234122884
C	35.79933940002607	-28.35260664525229	3.47402021088610
C	31.44708060733032	-24.6138469951139	3.47419377293649
C	33.95051357377725	-23.96832556924105	8.97915804247113
C	37.87187258317294	-28.43218325598950	7.73332575513880
C	35.59896674457454	-28.82018821114152	2.10648813943957
C	31.43396226534845	-23.86618789522654	4.62056768088401
C	34.91963637870569	-24.77007068935485	9.52153245565859
C	38.04247391275079	-29.00651572463374	6.50151498617298
C	34.46951032701696	-28.20097318577882	1.65243743278102
C	32.48594248780110	-24.40509168300099	5.47321380282803
C	35.29015460796288	-25.72114322241069	8.48446841938004
C	37.00633054222870	-28.44996601919756	5.64256919932958
C	34.00710102235314	-27.34885319447839	2.74222339421510
N	36.24042993426140	-27.55919618102068	6.33634260641579
Fe	34.66555917093125	-26.51688874100593	5.58998838207195
C	33.75753581211953	-31.51349897060983	7.10338326996574
C	35.18120121358089	-31.98747610326883	6.83412873278449
C	32.08406193375267	-27.60774980046411	7.00275871971078
C	33.37250066498991	-27.94202420080113	6.29513292512462
C	33.53016847426590	-29.36468451089515	6.03822809624158
O	33.49259156786739	-29.95927891361091	4.97521759588159
O	33.68325672683028	-30.09235274613703	7.22850029136938
H	29.80605225729812	-22.51215689724559	4.19917375108305
H	31.11549180109316	-21.78922248305644	5.14117559986459
H	29.98796294288995	-22.90603279159439	5.91234241462043
H	31.16375748637218	-24.21092555531700	1.36587028087175
H	30.06903084800845	-25.43068883636258	2.01990561858563
H	29.80836836750851	-23.72158161704797	2.38946384851728
H	33.67629358381420	-27.35819104323349	-0.17591118281463
H	34.36067592101995	-28.97792161185306	-0.35668830171691
H	32.78599894218024	-28.76304345943213	0.41755349445240
H	36.18527807729212	-29.93173589787803	0.35279347800756
H	37.53259312883707	-29.49627437660176	1.41124305893273
H	36.43460101246858	-30.80054117485988	1.87203128929455
H	33.57503166627088	-22.62665794319567	10.62775146432130
H	32.13989053245299	-22.99983957210334	9.66509099849481
H	33.35683750591588	-21.88865230481351	9.03534514927006
H	36.61194390998193	-24.55099896694798	10.85288038748132
H	35.37422130281242	-25.66195133904614	11.43996208568308
H	39.48965617728064	-29.34536322680424	8.83186204045654
H	39.09327778564284	-27.70753415359315	9.36759524976926
H	38.03907382427076	-29.05506748156286	9.79914512409366
H	38.59622612265543	-30.96723633997205	5.77455427137827
H	39.63499993665444	-29.66318493450428	5.19508930121863
H	39.78180875449097	-30.23494738453327	6.86191167521307
H	35.09183241667953	-23.91786012129987	11.49756631619259

H	35.86335988990498	-31.61153749577064	7.60170826562147
H	35.23148375725118	-33.08360745343568	6.82810665858958
H	35.51960494985037	-31.61760671500795	5.86490017414786
H	33.09058963800187	-31.84651402651844	6.30362796330440
H	33.39141015716224	-31.90519723060612	8.05849184673440
H	32.08421553658597	-26.59867955942416	7.41801021004188
H	31.22343421974884	-27.66666352378536	6.31280503764962
H	31.87222671548388	-28.30999265969735	7.82349931685745
H	32.34428466355057	-26.50655806222201	1.73264738481347
H	36.78745994708584	-26.74976039513662	9.58055116823052
H	37.51368404497224	-29.52314512446451	3.88962971185098
H	32.19256192283227	-23.08924289430817	7.10757032487641
O	35.84410620321245	-25.22530565276022	4.94079220968081
H	36.44810009913017	-24.98843262645650	5.66079990824778

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B3LYP Scan/Hydroxide IPC Model/Triplet/120 degrees Constrained Optimization

C	30.58362178823927	-24.43907794582805	2.24669298262510
C	35.50945121965224	-24.89838590973306	10.88417111281624
C	39.12831686364330	-29.97725557892874	5.88362242645343
C	33.80426658530786	-28.22507798849578	0.21331398058002
N	33.12102240911724	-25.45524434584198	4.81884239439919
N	34.57027393581455	-25.56788291342388	7.31189577550932
N	34.83157134534280	-27.45306486605736	3.73947525717779
C	32.91181931639887	-26.46070178533738	2.60172434953699
C	32.78190233216694	-23.98887114239566	6.75167170316033
C	36.30644321507374	-26.77043093240718	8.54646290234382
C	36.84381630260196	-28.77080086698057	4.17997611188519
C	30.54655720821332	-22.73270215374542	5.01661235224185
C	33.19407377518142	-22.97333771757225	9.65090650597348
C	38.72228051505488	-28.69441019631813	8.84975064320838
C	36.50405378208584	-29.70987118062924	1.25156302643440
C	32.52259020860555	-25.57136373677372	3.59916993255071
C	33.73262690759642	-24.53130499856312	7.61336336516015
C	36.76802421613678	-27.57710210567842	7.50948789398834
C	35.81277443739292	-28.31903193097344	3.36475399909777
C	31.45237978409579	-24.59295321569952	3.46034407924906
C	33.93920409834166	-24.09402019790440	8.98722207757869
C	37.91542016571737	-28.46749671957608	7.60510490344276
C	35.61359612034213	-28.75219721725906	1.98573666745025
C	31.44006899614799	-23.87213638695734	4.62414740530942
C	34.91289327081843	-24.90430809836206	9.50770247959055
C	38.08735275532364	-29.00618404538476	6.35719385391414
C	34.47752278901815	-28.13133715616448	1.54995221677611
C	32.49367823075115	-24.42888552722919	5.46217338244927
C	35.29816339842522	-25.81649371750611	8.44128329751651
C	37.03312889046383	-28.45052470416726	5.52102793020526
C	34.01071497379964	-27.31122153183239	2.66282274523997
N	36.25473990928589	-27.59425447263224	6.24416402295825
Fe	34.67453470609199	-26.54413417993499	5.52950997458414
C	33.61775785414840	-31.40634241554821	7.50096892316969
C	35.07160763593664	-31.82238798483455	7.69557784335954
C	32.00097928080183	-27.60484322361035	6.72283657858212
C	33.37953311424752	-27.96345812450639	6.22727504682376
C	33.65247833435456	-29.38602951287347	6.18555698976049
O	33.94789766987777	-30.08680906201336	5.23155095843070
O	33.47077784872486	-29.98820719712782	7.44640031850160
H	29.81184434433368	-22.50897824317010	4.23512826976150
H	31.11640616327814	-21.81141326707461	5.20254562037444
H	29.98746187927570	-22.95125939534849	5.93718040287374
H	31.16244434462712	-24.12665819509518	1.36571491518953
H	30.08449657913507	-25.38109591537049	1.98078915284284
H	29.80115294776781	-23.68859308557715	2.40472482617649
H	33.70455504526553	-27.24015557348142	-0.26407059806921
H	34.36712165321025	-28.86510511897191	-0.47514561767178
H	32.79131697039126	-28.64398278804309	0.29507109260841
H	36.19896201969910	-29.82109734818661	0.20505021948186
H	37.55085259170336	-29.37604338433509	1.25364346256450

H	36.48596444584719	-30.71009181460242	1.70638929547200
H	33.53932689408880	-22.81354748198703	10.67838462799598
H	32.11383990335429	-23.17119805331850	9.69560026436042
H	33.32028074792077	-22.02449207037932	9.11100228348707
H	36.59334639754896	-24.71747761486846	10.85860902479354
H	35.36118691697478	-25.85933852074130	11.39640361525205
H	39.54747836892966	-29.39266516678848	8.67186847097358
H	39.15981939088197	-27.76043931250528	9.23003896897664
H	38.11044810247105	-29.11187720563390	9.66166960652602
H	38.67938545362872	-30.91983543753021	5.54135798804787
H	39.70391695463118	-29.57324493224231	5.03931181265342
H	39.84155473278852	-30.22479373480813	6.67771716331574
H	35.06305379580427	-24.12080099559043	11.51377442016920
H	35.49499336988612	-31.34061304418530	8.58149437972823
H	35.15270752089739	-32.90981056837563	7.81823749135117
H	35.66312217561541	-31.5240491912034	6.82872856287679
H	33.21775564181147	-31.85270494172590	6.58644035953003
H	33.00519708309427	-31.72693863127683	8.35067373351371
H	31.99408544718489	-26.67249579416774	7.29581789223942
H	31.31936964078169	-27.44157297249714	5.87268676557420
H	31.55884286383958	-28.38921630885257	7.35062546529138
H	32.34486342908473	-26.44722317306989	1.67547742153208
H	36.80816481425994	-26.85954375267269	9.50548956481805
H	37.54661695636700	-29.47230145340153	3.74036651262142
H	32.18828453112170	-23.16356078601274	7.13402762385922
O	35.85366063585321	-25.24244215222141	4.89667416562326
H	36.42039703430465	-24.97311991496322	5.63527814625038

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B3LYP Scan/Hydroxide IPC Model/Triplet/130 degrees Constrained Optimization

C	30.57055085440731	-24.44799525766182	2.25173681604590
C	35.51017291488374	-24.94059831965983	10.87807716059235
C	39.14734694437900	-29.96493958777988	5.83524600606867
C	33.80267426860914	-28.21030500935798	0.18972559901079
N	33.12133476939172	-25.4643873986924	4.80978931624521
N	34.57760970477287	-25.58483865598839	7.29976296364450
N	34.83516023373363	-27.44978583746639	3.71715403072153
C	32.90291642916254	-26.46709438991541	2.59235355071209
C	32.79246084692900	-23.99953501446065	6.74570483521949
C	36.30803917298338	-26.79989553920855	8.52897416165921
C	36.86450220051249	-28.74608502273157	4.14038880979400
C	30.55109715893155	-22.73907885689832	5.02047714671690
C	33.20613782434723	-22.99851952483544	9.65019854073362
C	38.72318550605100	-28.72656863062902	8.81804437023241
C	36.52637664932249	-29.66675439252262	1.20659913685247
C	32.51643596924741	-25.58045536627935	3.59359086498010
C	33.74257083685895	-24.54728457312361	7.60498663544583
C	36.77271003640571	-27.59515796169111	7.48448206060479
C	35.82606416373179	-28.29979708554142	3.33206821390348
C	31.44541305697788	-24.60215099854437	3.46093407682549
C	33.94831488217920	-24.11827747539946	8.98164280832874
C	37.92206245609763	-28.48380555985523	7.57270830358458
C	35.62659474512414	-28.72556886513725	1.95084759937381
C	31.44071989873586	-23.88025132575898	4.62432783747106
C	34.91715559587654	-24.93588063683080	9.50006152274411
C	38.10134851556656	-29.00368317624659	6.31783668708655
C	34.48040983658103	-28.11671737410376	1.52418279473069
C	32.49847324162864	-24.43750981745908	5.45677087089089
C	35.30210347002522	-25.84278289215139	8.42918270024468
C	37.04830536242779	-28.44060935017219	5.48521495666969
C	34.00871784065707	-27.30939678807820	2.64452267811328
N	36.26369915809579	-27.59787952781801	6.21704619266140
Fe	34.67877023623991	-26.55301142930432	5.51364894936225
C	33.55826157393557	-31.40984270505461	7.51487957565643
C	34.98326631371824	-31.74195570733840	7.94516148517338
C	32.01224596271619	-27.60087897509710	6.72002591704061
C	33.38511972405595	-27.96924780298640	6.21703055156069
C	33.68435657921384	-29.38338664084844	6.21515475409181

O	34.13598607297897	-30.07073870531169	5.31251202096102
O	33.34118167008054	-30.00294397341037	7.43785455580005
H	29.80920475400065	-22.51862285089103	4.24487696277006
H	31.12257602793153	-21.81700551650610	5.19733707124946
H	30.00061215183511	-22.95395229762676	5.94705480822263
H	31.14290974993443	-24.12555518977090	1.37010488955872
H	30.07812658836719	-25.39250713111937	1.98239739111855
H	29.78253917205538	-23.70497175857450	2.41752209545597
H	33.67537070735073	-27.22204223988223	-0.27370634069932
H	34.37836494754698	-28.82637862378310	-0.50995299738206
H	32.80106819212105	-28.65615309998721	0.27007223369978
H	36.21670945763463	-29.77767986311619	0.16140328250455
H	37.56820485377796	-29.31769937103905	1.20439117883475
H	36.52576459519812	-30.66920122638382	1.65688846567034
H	33.55350353718180	-22.84260019558004	10.67755711567096
H	32.12563598141472	-23.19470267215987	9.69628921577602
H	33.33296293153993	-22.04822966097099	9.11306039954451
H	36.59521358797026	-24.76629658871886	10.85626699655052
H	35.35462484631108	-25.90314442417073	11.38518024223133
H	39.55029468202499	-29.42121934904667	8.63489423953142
H	39.15744106659989	-27.79730976059857	9.21335689326793
H	38.10767260716201	-29.15606482523757	9.62083758906007
H	38.70249634614753	-30.90478365265277	5.48054422841975
H	39.72334774734973	-29.54839364248640	4.99733904186193
H	39.85964110774648	-30.21910108966825	6.62810525588042
H	35.06689576614996	-24.16347477307799	11.51047214056609
H	35.22057965492844	-31.25768237450658	8.89702270415476
H	35.11239059623622	-32.82504509384878	8.06494792341816
H	35.69264865924158	-31.38762671032712	7.19561037632874
H	33.34059528669994	-31.86916937897370	6.54712310379208
H	32.83588239069517	-31.77538533741358	8.25311592622666
H	32.02038742183984	-26.68293137689827	7.31619228356973
H	31.34106364175562	-27.40006169172081	5.87062819731952
H	31.55345429749161	-28.39304572363125	7.32301811918206
H	32.33128661278760	-26.45367755157108	1.66900149005538
H	36.80742841534374	-26.89855083872745	9.48827092307009
H	37.57387831622639	-29.43636934637829	3.69370826383092
H	32.20144411829809	-23.17395187773359	7.13143538837502
O	35.84818571141890	-25.24237418335357	4.88235501595799
H	36.41393477211076	-24.97136234633947	5.62115661079992

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B3LYP Scan/Hydroxide IPC Model/Triplet/140 degrees Constrained Optimization

C	30.56962836923079	-24.44905627063735	2.26171811201930
C	35.52501057826325	-25.00094947520641	10.87499969356502
C	39.17749308610335	-29.95488017905773	5.77412161664232
C	33.81052925058655	-28.18067106731498	0.16071462317514
N	33.12735563450217	-25.48015462837682	4.80671704692458
N	34.58984371316649	-25.61650931528548	7.29226782140077
N	34.84213848961950	-27.45424559546626	3.69552818588638
C	32.90282722509903	-26.47034446731701	2.58388278528499
C	32.80250370849130	-24.02838016498773	6.75300534733480
C	36.32268185205200	-26.83993503564395	8.50946084069818
C	36.88925153692845	-28.72823339014699	4.09743859341099
C	30.56014152895700	-22.75367955152997	5.03829398599568
C	33.21730893402962	-23.05153419580204	9.66557417916127
C	38.74583374830552	-28.76075928589234	8.77498580883634
C	36.55396635801629	-29.61839218496727	1.15345533273277
C	32.51893290861078	-25.58964767290917	3.59157207256067
C	33.75389087668811	-24.58217696994683	7.60690766207084
C	36.78954792258972	-27.62203313230756	7.45588154034374
C	35.84210526026062	-28.28762824744418	3.29775488611981
C	31.44751859809208	-24.61082027959043	3.46779309002990
C	33.96026481141031	-24.16476995282942	8.98700146167779
C	37.94364419418448	-28.50614485097551	7.53267927948010
C	35.64316632543670	-28.69961620511815	1.91221478563816
C	31.44673445326704	-23.89481293745911	4.63504788675361
C	34.93057610508170	-24.98552118316560	9.49770654544434

C	38.12690768306677	-29.00593744895128	6.27029482764811
C	34.48871891931391	-28.09893461011920	1.49573927556011
C	32.50653941249079	-24.45685362738394	5.46125546202883
C	35.31579066351631	-25.88287395964133	8.41899203586373
C	37.07095843885881	-28.43769840414591	5.44537096901786
C	34.01243398100187	-27.30823301926126	2.62590549984099
N	36.28137136141538	-27.61061978703369	6.18856947129545
Fe	34.68904030147582	-26.57265123675458	5.50006227827765
C	33.47643814491777	-31.42525051909070	7.54270542807382
C	34.79665829289145	-31.66827192409777	8.26706015035790
C	32.01968230731312	-27.62113266741522	6.66828716969291
C	33.40282086411334	-27.99548691606537	6.19764739667415
C	33.72940134103488	-29.40017069194294	6.25644543214181
O	34.35282640403420	-30.07595427744841	5.45102814080884
O	33.19987407596623	-30.03516695566373	7.40674079689863
H	29.80150074897414	-22.54443577677557	4.27591917690341
H	31.13077349907910	-21.82712584358781	5.19391970550604
H	30.03007118030732	-22.96159037622952	5.97808394645267
H	31.13585271250130	-24.10008548515651	1.38614417398374
H	30.09381499532291	-25.39676029195861	1.97478731102537
H	29.76883925800036	-23.72309972902811	2.44150377290823
H	33.71459263549757	-27.19215656518531	-0.31026668267161
H	34.36800582849865	-28.81901653395852	-0.53364352312530
H	32.79550832352857	-28.59439022388242	0.24266845181268
H	36.21978137033996	-29.75228830772164	0.11859080248453
H	37.58285361805696	-29.23382978252405	1.11854955741359
H	36.60052261430899	-30.61442822510058	1.61506292276611
H	33.54779609480949	-22.92010624297199	10.70187758361647
H	32.13463492350466	-23.23870097464527	9.68892912890654
H	33.36176186698924	-22.09132558483431	9.15074946637652
H	36.60928552227995	-24.82176118270306	10.85355681760252
H	35.37430324356384	-25.96894114439965	11.37308433561716
H	39.57328487064947	-29.45300861647263	8.58431913844881
H	39.18014620790213	-27.83509678360979	9.17876732727028
H	38.13105567543705	-29.19820024858045	9.57393176071888
H	38.73447173784503	-30.88539921802464	5.39395064699187
H	39.76057694981137	-29.51875468267771	4.95106073841762
H	39.88303112812547	-30.22766937364246	6.56680127842107
H	35.07928005480396	-24.23172027023748	11.51523785092429
H	34.79900759872111	-31.16418615734421	9.23821539871905
H	34.96185963541112	-32.74053614586583	8.43118528099623
H	35.62672661849901	-31.27641508447269	7.67629896943964
H	33.49585517036559	-31.89480692382700	6.55602884809151
H	32.63908468933594	-31.83679296753797	8.11754948133582
H	32.02425508677145	-26.71577346203663	7.28429524411138
H	31.37990900045705	-27.38876183791606	5.80415163954283
H	31.53183222745150	-28.41806515911666	7.23878023043054
H	32.32884426053938	-26.45125452112381	1.66208946533714
H	36.82264474362573	-26.94720284809909	9.46752733202196
H	37.60590210618010	-29.40445713510449	3.64093461020758
H	32.21211755593509	-23.20557559078897	7.14558508116546
O	35.85266001695616	-25.25512503804635	4.87146097843763
H	36.41010772223012	-24.97660692341887	5.61378357602348

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B3LYP Scan/Hydroxide IPC Model/Triplet/150 degrees Constrained Optimization

C	30.56411448348363	-24.48936441820279	2.25174910674411
C	35.50404645089242	-24.91825635233141	10.88050971488452
C	39.19394227609330	-29.91098783285984	5.84379674335676
C	33.83289935360857	-28.22375124195791	0.19934154175609
N	33.12204805764066	-25.47968031734194	4.81294854471025
N	34.58046794218796	-25.58068410450330	7.30381424159332
N	34.85712091186455	-27.44364582561393	3.72467990221026
C	32.90653822897148	-26.49496493414456	2.60226797527488
C	32.79617906285862	-23.99851522728090	6.73717767114178
C	36.31162384677857	-26.78734880872953	8.54048283523644
C	36.91467138010003	-28.69629947707706	4.14242500598831
C	30.55347112981010	-22.75004519683287	5.00153802005514

C	33.20405288649643	-22.98211715990492	9.63610435031954
C	38.73569053340120	-28.70389549423153	8.83503505110512
C	36.59542811295473	-29.61304790418822	1.20572731097167
C	32.51484109178902	-25.60650125560430	3.59929644562934
C	33.74493420420954	-24.54112731270035	7.60081668333880
C	36.78972528808688	-27.57285554643746	7.49479906810877
C	35.86749151470114	-28.26816582024834	3.33567254386665
C	31.44219538966926	-24.63070909286668	3.46016365262250
C	33.94653114402913	-24.10637915108902	8.97544007048980
C	37.94470854797422	-28.45430219780807	7.58462353015171
C	35.67523085758341	-28.69516479594479	1.95413573303245
C	31.44056915252605	-23.89666669463337	4.61561779816896
C	34.91330587798312	-24.92236990095407	9.50145368139193
C	38.13885229894233	-28.95997101800872	6.32636462611736
C	34.51302514161329	-28.11411880657454	1.53152814966907
C	32.50080794243115	-24.44593890607951	5.45149771888899
C	35.30231420163658	-25.83340719906543	8.43603041296889
C	37.08771421876535	-28.39818582844503	5.49016200549881
C	34.02565691500421	-27.31946348224150	2.65404677468724
N	36.29085991011176	-27.56850215396536	6.22317696866029
Fe	34.68919047186504	-26.55145592342283	5.52221760525393
C	33.34132456229191	-31.51780115922958	7.25777906866075
C	34.68292616280932	-31.94356524168607	7.84590767633781
C	32.20267353276279	-27.60684980296908	7.03380621534258
C	33.43424221183061	-27.98018308884376	6.24520809535612
C	33.69885429383105	-29.39632983650932	6.16701448540189
O	34.24877626211349	-30.02974278710438	5.27641844636949
O	33.17702894102678	-30.10373367697535	7.27835638828158
H	29.80848563943595	-22.53854555647448	4.22639190130598
H	31.12677539272081	-21.82647165738365	5.16427057525360
H	30.00674232777176	-22.95241762131057	5.93311123516207
H	31.13426567356213	-24.17634775402779	1.36531292303253
H	30.07105324993558	-25.43671326768142	1.99374251585189
H	29.77657456846184	-23.74452432171243	2.41159147151560
H	33.66264786222980	-27.23756241533390	-0.25435073419635
H	34.42998465905775	-28.80934716742180	-0.50862143939303
H	32.85088974749377	-28.71132554025132	0.28027568311127
H	36.28250144798592	-29.73381443089095	0.16259585779497
H	37.62757960775126	-29.23632772893896	1.19706099798461
H	36.62402588163495	-30.61441657981389	1.65745460034756
H	33.54250971005464	-22.82682969639546	10.66652412708597
H	32.12231038305110	-23.17308223001556	9.67221597688412
H	33.34053935437283	-22.03298825163867	9.09924218448788
H	36.58788857448479	-24.73637578920921	10.85981257567102
H	35.35456255802451	-25.87997931681797	11.39097889478325
H	39.56830000377580	-29.39237125083875	8.65345005492424
H	39.16122262519696	-27.77581451846703	9.24250187715344
H	38.11504155124880	-29.14350160839370	9.62836933341907
H	38.75578387459349	-30.84725505488197	5.47192226580783
H	39.77833299770385	-29.48198408066690	5.01797739178876
H	39.89779821198705	-30.17312910573977	6.64158411807755
H	35.05434234696248	-24.14198654747877	11.50935930307319
H	34.80082667156960	-31.54965402317844	8.85995012953433
H	34.76240941801134	-33.03717772010848	7.88752072595240
H	35.49854821962154	-31.55949238044963	7.23094782352370
H	33.24860020318022	-31.88311714400090	6.23167308667424
H	32.51363795230779	-31.91683087864170	7.85478680172626
H	31.80793924533618	-26.63794251226358	6.72790476171914
H	31.40139394854623	-28.35208315401142	6.94952567949034
H	32.42883071859248	-27.52670569384411	8.10936136086977
H	32.33295076371168	-26.49220734439337	1.68004589816337
H	36.80534916207926	-26.88619846385746	9.50271662213691
H	37.63753645029856	-29.37097853936502	3.69348615248930
H	32.20532339205092	-23.17004485422260	7.11693789114206
O	35.83420422919791	-25.22059846442516	4.88907604849659
H	36.44112573626921	-24.98934590384548	5.60846080951053

B3LYP Scan/Hydroxide IPC Model/Triplet/160 degrees Constrained Optimization

C	30.53908457082301	-24.53737730295327	2.28372009854081
C	35.53479397887915	-24.90762443697245	10.88136938887023
C	39.26086006884334	-29.84162801415431	5.81828115983204
C	33.82171117193677	-28.25799618332423	0.22234682342352
N	33.12691491033453	-25.49501390423361	4.82665708392795
N	34.59639761179358	-25.58331083419819	7.31134867478767
N	34.87095484785713	-27.44589564119707	3.73266156686369
C	32.89537220316169	-26.52956873591200	2.62674835846770
C	32.81269729459684	-24.00094895235262	6.74322325947243
C	36.33961433602320	-26.77847190575346	8.54127248832473
C	36.95936876992842	-28.65272174582535	4.13105959133990
C	30.55486228077681	-22.76930362274028	5.01545546125142
C	33.23241664499728	-22.97359144887708	9.63825885405496
C	38.78945713112059	-28.66466078539830	8.81955169008983
C	36.62581107770713	-29.58466294181848	1.19983900992188
C	32.50794114187310	-25.63525884787990	3.62064372203653
C	33.76324643504130	-24.54128752293407	7.60674544087084
C	36.82462556056300	-27.55273221740998	7.49031092921215
C	35.89460654372440	-28.24958950876825	3.33450682205658
C	31.43117237755687	-24.66361818652957	3.48343060629164
C	33.97056365005144	-24.10154410991882	8.97906457954651
C	37.99332662209481	-28.41722641532790	7.57191387840861
C	35.69509890197665	-28.68414010560597	1.95642053172537
C	31.44037416249367	-23.91772897701190	4.63130505269197
C	34.93822346626783	-24.91671814048414	9.50479447508918
C	38.19398193494479	-28.90852490398630	6.30926585134521
C	34.51541768632465	-28.12939573396179	1.54585289487095
C	32.50967265177484	-24.45699053826506	5.46202795671484
C	35.32351471284196	-25.83126698151325	8.44112018617579
C	37.13242348049010	-28.35746675210839	5.47911848803864
C	34.02558775378586	-27.33971194529852	2.67070940541200
N	36.32391950959067	-27.54646563925290	6.21970556700431
Fe	34.70500708140485	-26.55420936434964	5.53010886289421
C	33.20896833062787	-31.55359614224075	7.13543605594067
C	34.44751720864488	-31.96716084561908	7.92484001521014
C	32.20067561333598	-27.62368430122360	6.99288932308298
C	33.46169364702998	-27.98871754399222	6.24871390936121
C	33.73417632561540	-29.40310602564202	6.18392811631609
O	34.45489624449582	-30.01533214850818	5.40578542116751
O	33.01018651675145	-30.14470471765537	7.15281281510156
H	29.80521653034204	-22.56272010299621	4.24351441972388
H	31.12878403480435	-21.84465034542807	5.16948216333035
H	30.01360092265853	-22.96640516088137	5.95137948304141
H	31.10128553771373	-24.25008398321706	1.38370557221505
H	30.03157541390137	-25.48406512799390	2.05218041805728
H	29.76237811083629	-23.78007130841532	2.43775557944003
H	33.63835188279531	-27.27795914908618	-0.23965124831278
H	34.41569529430014	-28.84611955416799	-0.48613269123211
H	32.84463105930455	-28.75244596963812	0.31915335272752
H	36.29669689317651	-29.72518198102771	0.16419576461631
H	37.64692498433278	-29.17999431577475	1.16770861719420
H	36.69070177572501	-30.57979117476539	1.66140861753735
H	33.57424390115235	-22.81592375279866	10.66722501267430
H	32.15034512256387	-23.16192943484323	9.67812468890403
H	33.36956924286709	-22.02638298637859	9.09815333983454
H	36.61845813778243	-24.72529490707106	10.85544020133369
H	35.38812283043686	-25.86768831704536	11.39581839899588
H	39.62777078511139	-29.34498065315227	8.63335452791310
H	39.20781181614866	-27.73449746546976	9.22988055230395
H	38.17455729529993	-29.11279632703264	9.61256375987918
H	38.83329104122184	-30.78065060117813	5.44112618135604
H	39.83788567043762	-29.39942323780391	4.99420865952719
H	39.96977091292306	-30.10000116315593	6.61285363277455
H	35.08747134486210	-24.12945528972813	11.50958140920463
H	34.39049993925801	-31.59707077692850	8.95320433000359
H	34.54473792784430	-33.05970182433092	7.95487103111111
H	35.34201678014242	-31.55200343306952	7.45767534736821

H	33.29097629708339	-31.90121814555076	6.10213449559754
H	32.30467140046591	-31.97986355552123	7.58379032254705
H	31.91470476829135	-26.58577240728273	6.83528534584031
H	31.35253571648578	-28.26161742530594	6.70843730154777
H	32.32525492838069	-27.76655005484688	8.07777598478604
H	32.31196974606812	-26.53896378181898	1.71071411617579
H	36.83745255713803	-26.87527165319647	9.50161667750801
H	37.69326241125663	-29.31093819331948	3.67555757263807
H	32.22417544951423	-23.16992090638021	7.12102435306393
O	35.82788424463381	-25.20656938438123	4.89164250564980
H	36.44249198765728	-24.97465562081896	5.60429512938905

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B3LYP Scan/Hydroxide IPC Model/Triplet/170 degrees Constrained Optimization

C	30.53162100763857	-24.57836099322857	2.33694848228844
C	35.57601961036910	-24.87195225546628	10.90683870995677
C	39.31911457890450	-29.79413160086278	5.85944213246862
C	33.84155264498924	-28.29293349559075	0.27440492979493
N	33.16664166316294	-25.48268945185336	4.85284575358028
N	34.61231382149058	-25.58149912354586	7.35128106595141
N	34.91035303990984	-27.42832391748512	3.766635111110971
C	32.91903701730020	-26.53785132078414	2.66252950988900
C	32.83889219251797	-23.99400571448263	6.77395303427248
C	36.36283469552903	-26.76423948377312	8.57743681429826
C	37.00001350553297	-28.63504813658061	4.17299415644537
C	30.54878300433637	-22.80149313336510	5.06288028585100
C	33.27423972203172	-22.94098751574227	9.65762889213056
C	38.83234186011893	-28.62046487247222	8.86030291897204
C	36.65586667750365	-29.59511935355061	1.25145962241155
C	32.53063042746219	-25.64076923442292	3.65430184116390
C	33.79073984701486	-24.53123516505228	7.63755622464568
C	36.85121355586734	-27.53759237975072	7.52848589790560
C	35.93409852494545	-28.23872816302484	3.37369404973408
C	31.44101338607421	-24.68514495719529	3.52580929280659
C	34.00445086414319	-24.07860670772843	9.00661573785659
C	38.03291525739733	-28.38785522485898	7.61223404635048
C	35.72883715340298	-28.68652624861279	2.00326675300576
C	31.45128351778430	-23.93462293267105	4.67217550797980
C	34.97037226869700	-24.89230925488044	9.53457179813345
C	38.23924395047038	-28.87730967097089	6.35168477396873
C	34.54313503780415	-28.14106647141125	1.59165436266796
C	32.53456965282000	-24.45410451210545	5.49443905281049
C	35.34739543279453	-25.81748597216081	8.47430491418597
C	37.16694306032005	-28.34049316515435	5.52172223582540
C	34.05428828275400	-27.34268669563447	2.70755191179618
N	36.34615866779448	-27.54682185544651	6.26300121310052
Fe	34.73837819873854	-26.54903059673838	5.57336888457766
C	33.06478268984740	-31.58805026335448	6.90734766516301
C	34.23330393040280	-32.08498475654228	7.75360616683803
C	32.28994635016085	-27.59327417106794	7.11896932441402
C	33.48732405061519	-27.97958023416173	6.28685726122822
C	33.71418825390855	-29.39596221184523	6.14921659848051
O	34.49660810527956	-29.97972801333292	5.40788176651374
O	32.89404782813764	-30.17893732355844	7.00286153287919
H	29.80003952028587	-22.59705834921732	4.28948431010104
H	31.10951021345633	-21.87096131202981	5.22919878500524
H	30.00579249934123	-23.01495506723439	5.99415722697631
H	31.07976333379163	-24.30493880174424	1.42393862440009
H	30.02192598064751	-25.52904875986995	2.12768209134094
H	29.75627419087801	-23.81955847656942	2.49009206851375
H	33.61154660999040	-27.31978886337095	-0.18105920096463
H	34.45214123253157	-28.85244291275005	-0.44311808576544
H	32.88734958156154	-28.82888187016036	0.37893699985656
H	36.33625565642826	-29.72548909199499	0.21148634475266
H	37.68261328815704	-29.20449732595943	1.23303603490761
H	36.70208898201379	-30.59358059479564	1.70798028619951
H	33.60980294754562	-22.78551422923058	10.68900137119328
H	32.18971200196482	-23.11676437146508	9.68955831093076

H	33.42671765407361	-21.99631200362867	9.11715086816552
H	36.65571242031587	-24.66887512497090	10.87285455395134
H	35.45091895736211	-25.83457435613658	11.42214684407593
H	39.67467998053770	-29.29700693193345	8.67826768339581
H	39.24500055297378	-27.68421188110876	9.26218955951940
H	38.22125569317284	-29.06614969408723	9.65778958544911
H	38.90483410980212	-30.73596092508484	5.47419260737446
H	39.89467609361304	-29.33938667314805	5.04112385805624
H	40.02746533745542	-30.04907699737828	6.65566239643456
H	35.11827049064645	-24.10230615591446	11.53812905620786
H	34.11094114568527	-31.78066257070402	8.79774312452309
H	34.30218089883429	-33.17956756699270	7.71873363977029
H	35.16800330596343	-31.66598467036824	7.37801559821779
H	33.21415067654090	-31.87127018878024	5.86181777888410
H	32.12114052492694	-32.01835251863025	7.26071750987284
H	31.93950867198484	-26.58897714761399	6.88460804821543
H	31.45266612478235	-28.29173547922549	7.00659484401783
H	32.54481422948270	-27.59256409147035	8.19101417961178
H	32.32733385190915	-26.56160274664576	1.75218727900284
H	36.86579947557876	-26.85201730342755	9.53606033670209
H	37.73845457737163	-29.28899930665233	3.71871839934925
H	32.24818201528108	-23.16383345087487	7.15019991590360
O	35.89284250668207	-25.20673145490571	4.98035454530212
H	35.61905048345686	-24.94993772645863	4.08689172909699

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B3LYP Scan/Hydroxide IPC Model/Triplet/180 degrees Constrained Optimization

C	30.50108933408931	-24.65510288756742	2.39284216738451
C	35.64433356748339	-24.81443801912693	10.90647828143827
C	39.42088811813606	-29.68718887864465	5.84522454465521
C	33.82552592038252	-28.35792556246243	0.32978969514309
N	33.17593879266654	-25.50493339747071	4.88565211701527
N	34.64473454120684	-25.57046904000823	7.37036257856500
N	34.93122184555876	-27.43892430834545	3.79593926508596
C	32.91134847735973	-26.58900150728247	2.71129276187429
C	32.85765901093541	-23.99768485253988	6.79363084278908
C	36.42537268958510	-26.71827739911141	8.58520399398653
C	37.05168327808379	-28.59716681502270	4.18318286141133
C	30.53993331667226	-22.84215924061255	5.09467367628744
C	33.31778413662352	-22.91067172747247	9.66165020001195
C	38.93715377944336	-28.51753141984946	8.84775714060038
C	36.67749305700435	-29.60027192573547	1.27719910204766
C	32.52630525787409	-25.68383282543365	3.69719057229466
C	33.82034708555280	-24.52117868607944	7.65396445564176
C	36.91786481176315	-27.48508846108048	7.53344174314068
C	35.96390158519247	-28.23497429596003	3.39647090639397
C	31.42739335935363	-24.73861856309134	3.57043971793252
C	34.04611692984489	-24.05236885933527	9.01565756739589
C	38.12041407900475	-28.30719721366662	7.60702550158198
C	35.74539353215258	-28.70122869290827	2.03429059928873
C	31.44639487514632	-23.97304215846750	4.70674338719542
C	35.02255719583969	-24.85447912816987	9.54182630338242
C	38.32524360009518	-28.79415231734065	6.34584964547339
C	34.54388182422721	-28.18074844549824	1.63486482764760
C	32.54324052846012	-24.47395149496461	5.52229717719920
C	35.39458634330465	-25.78804387250003	8.48734927165817
C	37.23073290745550	-28.28629374321585	5.52630511846131
C	34.05820717727057	-27.37804608061675	2.74859677855411
N	36.40023218951495	-27.50923428546875	6.27401441177911
Fe	34.76831083750615	-26.54671980760094	5.59668468525671
C	32.90015174336776	-31.60626285219405	6.65329640961833
C	33.83039313755007	-32.18248834677492	7.71709855674463
C	32.29481844682717	-27.62948726010202	7.08044960043815
C	33.53450085441469	-27.99366946069469	6.30129830751916
C	33.75576532100003	-29.40943705499451	6.14805664870109
O	34.66825070173891	-29.99097787197672	5.57126182071285
O	32.75336795541449	-30.19715420175104	6.77420118467654
H	29.78742417828868	-22.64502010238931	4.32303296152983

H	31.09708670880859	-21.90835123617853	5.25423064497355
H	30.00108906261092	-23.05309270714300	6.02900459533731
H	31.03796213204420	-24.41156731626281	1.46492534642358
H	29.97940611162335	-25.60611500638544	2.21660883432392
H	29.73504139261541	-23.88517142210500	2.53694577586808
H	33.58611581595781	-27.39350140330388	-0.13934062961345
H	34.42839812736160	-28.92774930961546	-0.38607687905152
H	32.87459799573649	-28.89482314758623	0.45631602260652
H	36.33194200832654	-29.76574913546425	0.25062103043454
H	37.69106726619751	-29.17992441965566	1.21905058640420
H	36.76741691567084	-30.58513722274844	1.75594869983497
H	33.66508590554648	-22.74103385779859	10.68689244252684
H	32.23456525009942	-23.09119474205686	9.70887474928957
H	33.45907629925830	-21.97191453925143	9.10794591787228
H	36.72203860874226	-24.60406686815113	10.85730671511713
H	35.53242952543073	-25.77217374285521	11.43381439802653
H	39.78740731668925	-29.18305103414820	8.66179606544221
H	39.34028202900135	-27.57210250164441	9.23788797868786
H	38.34139691710207	-28.96565965072880	9.65539785976088
H	39.02377441362160	-30.63820963644761	5.46456945623490
H	39.97970770306447	-29.22095123086640	5.02169369618330
H	40.14123544663757	-29.92585734409530	6.63575702526207
H	35.18857113930233	-24.04112615561190	11.53471816122736
H	33.48545471933987	-31.91032783682512	8.71955449175372
H	33.86874924200134	-33.27715604737192	7.65135547149489
H	34.83973644880620	-31.79157511885021	7.57917296158815
H	33.27490450484143	-31.85398449151817	5.65634539414336
H	31.88898544170638	-32.01330678631638	6.76416862545731
H	32.09823924544638	-26.56008702004045	7.07164055036251
H	31.40401745594438	-28.14557878421800	6.69723056226834
H	32.38237472958964	-27.94189567493199	8.13275160556654
H	32.30728876604744	-26.63097502805615	1.80972338988738
H	36.94030136593670	-26.79229940964354	9.53862091004620
H	37.79838505107360	-29.23801687184552	3.72367979352785
H	32.26614577641340	-23.16660221302707	7.16664385937831
O	35.89718534694916	-25.19079760564588	4.98601954260917
H	35.59949064406295	-24.93501396107722	4.09991630222938

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B3LYP Scan/Hydroxide IPC Model/Triplet/190 degrees Constrained Optimization

C	30.47205540134599	-24.74335328102135	2.44921321315710
C	35.73911393955645	-24.70894949316812	10.89409348617931
C	39.49403925887456	-29.62024893429295	5.85849425995710
C	33.81651387730122	-28.42922437171359	0.39518359634522
N	33.17216373368044	-25.54118473602531	4.93193306681575
N	34.68240117024272	-25.54729586649855	7.39384422544254
N	34.94683143134656	-27.46168868978265	3.84126712208181
C	32.90455587749120	-26.64786317088279	2.76906219535917
C	32.86016385928870	-24.01227233880086	6.82236251402798
C	36.50237354377170	-26.64553931578153	8.59468780894655
C	37.08821249383042	-28.58654075750049	4.21489358905182
C	30.51023547773709	-22.90431893719517	5.13325771911688
C	33.36128857093296	-22.86178687910812	9.65834687379563
C	39.03636978808832	-28.41297971141721	8.84955472649444
C	36.68918060932434	-29.63146531437607	1.32587323190080
C	32.51554324014962	-25.73923723509741	3.75045871996607
C	33.84720313384695	-24.50516818042399	7.67327936297558
C	36.98883138964862	-27.42132903294788	7.54716376254843
C	35.98423464428357	-28.25077347166189	3.43858857658966
C	31.40503931660922	-24.80784269851667	3.62284427134242
C	34.09247596490628	-24.00672333474237	9.02132315446437
C	38.20215263299357	-28.22803898312331	7.61650929412527
C	35.75595775332695	-28.73445975416966	2.08427895150547
C	31.42406221259404	-24.03132765500413	4.75175352587798
C	35.09084415549601	-24.78418887509401	9.54330109678588
C	38.39583090314432	-28.73098607202983	6.36028898311342
C	34.54516868308822	-28.22994584507644	1.69155467963925
C	32.53345822375669	-24.51117634360053	5.56298932179746

C	35.45640011225547	-25.73212484880797	8.49940359530912
C	37.28383549457600	-28.24880320537264	5.54887662962882
C	34.06175649491271	-27.42176194129999	2.80198325220259
N	36.45434279249086	-27.46972971586037	6.29551706275376
Fe	34.79427589708649	-26.54642345261800	5.63260011701974
C	32.78086341022376	-31.59891782864930	6.33989406614058
C	33.44976636637456	-32.27158886594894	7.53546481994828
C	32.31334120357342	-27.65164323115905	7.10090737752552
C	33.57944140183984	-28.00233496601548	6.35777645650731
C	33.78568652714590	-29.41472658792458	6.15688593922787
O	34.78104468482349	-29.99943847022199	5.74492644497369
O	32.65341232660562	-30.19368615767593	6.51499154657578
H	29.75301555043619	-22.72021901496895	4.36296229905593
H	31.06088035455281	-21.96484171878849	5.28156904374508
H	29.97697879359724	-23.11061419980829	6.07181647969063
H	31.00298401300910	-24.50633862373801	1.51617428617614
H	29.95567112151258	-25.69946583884391	2.28541237137043
H	29.70185240718804	-23.97671673758406	2.58858726760896
H	33.52552333541882	-27.47277415741839	-0.06030695358437
H	34.43530292871112	-28.96293560932353	-0.33492211243622
H	32.89379226589536	-29.01187997356498	0.52909022912301
H	36.34129137687121	-29.79927530754172	0.30042155930744
H	37.70111870492219	-29.20790460456304	1.26454278631076
H	36.78390630414212	-30.6158055035345	1.80499102183698
H	33.73507498077276	-22.65868760826566	10.66806405955230
H	32.28327110254970	-23.05989236285975	9.74191646255735
H	33.46958258050118	-21.93619148391231	9.07589051737116
H	36.81338234698765	-24.48920000537415	10.81889527793021
H	35.64744605387864	-25.65645293575923	11.44342044210525
H	39.88467377713930	-29.08124756848742	8.66452628499727
H	39.44371032858318	-27.45996478594753	9.21633831766917
H	38.45212973864120	-28.84647920936878	9.67334328533414
H	39.10101597551707	-30.57901445149357	5.49341343756350
H	40.04040674281680	-29.15922796416540	5.02365898668521
H	40.22466116302310	-29.84347382403543	6.64410648971680
H	35.28761193130068	-23.92718801017012	11.51487185563619
H	32.90882702752480	-32.04428027253697	8.45935199467149
H	33.47246669122798	-33.36129321393084	7.40868276821691
H	34.47569017708703	-31.91386600516200	7.63649274165645
H	33.34955247734727	-31.80693444698346	5.42930722098517
H	31.75745309589507	-31.96876311093308	6.21304656249603
H	32.28070182812137	-26.60394883070832	7.39212532884287
H	31.42477137387114	-27.84888480537380	6.48106238477871
H	32.18246393086758	-28.26411502522773	8.00303128530880
H	32.29307994959365	-26.70535731687671	1.87337773463439
H	37.03342269121266	-26.69752973518129	9.54068097869444
H	37.83596215467927	-29.22572094232478	3.75482941774165
H	32.26246088100935	-23.18420318640379	7.19228158771439
O	35.87984494998676	-25.16871982911817	4.99414771837823
H	35.56246004804218	-24.92508672529572	4.11146928534059

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B3LYP Scan/Hydroxide IPC Model/Triplet/200 degrees Constrained Optimization

C	30.45522137832202	-24.77448750360741	2.46777353600689
C	35.74951716167249	-24.69922640517103	10.89236409146327
C	39.50782865636258	-29.61300778112282	5.85739783165044
C	33.81200707962049	-28.44676732259928	0.40689337951435
N	33.18260109000277	-25.53698428827798	4.93166616574516
N	34.69769189513232	-25.53530378772711	7.39011848843883
N	34.95771701611317	-27.45926272448369	3.84172934339111
C	32.90764110665333	-26.65589395783027	2.77605473576513
C	32.86854878564810	-24.00750960767979	6.82123284117441
C	36.52275769013593	-26.62721952884008	8.58877977260247
C	37.09910571140139	-28.58443700657109	4.21518852829117
C	30.49584173462639	-22.92653059564713	5.14583794815795
C	33.36445723935014	-22.86006206412863	9.65982887730234
C	39.05634357363533	-28.39456624161176	8.84473521682489
C	36.68897882354505	-29.64453017766508	1.33222135073246

C	32.51922572899398	-25.74511549794738	3.75569015680857
C	33.85901056012420	-24.49619483263032	7.67064566329910
C	37.01080434246249	-27.40089709586585	7.54052323628210
C	35.99311380503645	-28.25161367090098	3.43987011367532
C	31.39955282037873	-24.82400995356795	3.63299921607026
C	34.10218494653709	-23.99890764543482	9.01948877323003
C	38.22285160896501	-28.20966092455126	7.61122616057842
C	35.75872799669171	-28.74345108907414	2.08956425546237
C	31.41960729235512	-24.04360971874927	4.75919981102892
C	35.10326268370771	-24.77351057268425	9.54055381537988
C	38.41367881396360	-28.71751375284775	6.35682197052999
C	34.54648543326238	-28.24026278241733	1.69882584373846
C	32.53901784731788	-24.51100218684533	5.56416561946366
C	35.47279076434523	-25.71822512450348	8.49520018054169
C	37.30151233928385	-28.23545381285707	5.54525487163031
C	34.06760743142990	-27.42589233285587	2.80639595091759
N	36.47596712140969	-27.45009902180767	6.28923441551174
Fe	34.81048410091366	-26.53452607647007	5.62926005907272
C	32.77552326843419	-31.58568323301534	6.23338454290319
C	33.29791330314164	-32.26098142831215	7.49830560717958
C	32.36089997903165	-27.65805544586392	7.15125175846803
C	33.59863301310583	-27.99675705558943	6.35590884898379
C	33.81147192294681	-29.40919847878061	6.15861806054377
O	34.84304221689748	-30.00210045790901	5.86643853502504
O	32.64153917565259	-30.17840836553248	6.39237160260930
H	29.73087303123336	-22.75219540467485	4.38094845118030
H	31.03660535744094	-21.98055062190461	5.28923810565426
H	29.97189599274445	-23.13798476605945	6.08847307428426
H	30.97651261969011	-24.54638789908983	1.52717517945106
H	29.93980237039599	-25.73367059842879	2.31941791512543
H	29.68436282506679	-24.00834732367774	2.60627382493587
H	33.53301506667574	-27.49262622466779	-0.06093391257624
H	34.42134866546493	-28.99897566645086	-0.31732505254493
H	32.88168765300362	-29.01457142229560	0.55114724325719
H	36.33328610701109	-29.82365319866797	0.31138833792169
H	37.69880649338153	-29.21791986887112	1.25841518328899
H	36.79160918587390	-30.62379846354263	1.82003263787630
H	33.73141610818311	-22.66318195320152	10.67328258072936
H	32.28655364160436	-23.06173062277231	9.73541168058355
H	33.47373612504963	-21.92990503412203	9.08481083296088
H	36.82058300833040	-24.46310337154905	10.82018266907801
H	35.67115346940196	-25.65234972092610	11.43386347498095
H	39.90505347098165	-29.06241522855281	8.66008975175249
H	39.46305412046660	-27.44156131947589	9.21224596583205
H	38.47161005900121	-28.82871914309174	9.66785267915045
H	39.11060210277172	-30.57247451645889	5.49878820488159
H	40.05382963862658	-29.15846926905282	5.01877806745561
H	40.23950010685169	-29.83428271054333	6.64259778379223
H	35.28613202769832	-23.92921581480195	11.51903624726918
H	32.66116211252261	-32.02130128416147	8.35550603199781
H	33.32009499995625	-33.35150744043928	7.37875838766756
H	34.31120420546327	-31.91584793942308	7.71010394315765
H	33.44282676605430	-31.79970832042651	5.39402071294633
H	31.76991630000039	-31.94623828024710	5.99085690958918
H	32.27424140387388	-26.59284601950464	7.35236000366771
H	31.44872961299226	-27.97120400722999	6.62212504739032
H	32.33746712209705	-28.18749568170305	8.11533443711888
H	32.29058489864359	-26.72167910796880	1.88476482038470
H	37.05412173096013	-26.67863707230767	9.53463742163878
H	37.84385218009491	-29.22851733865286	3.75709121555679
H	32.26728666185703	-23.18257626117661	7.19243142240309
O	35.88825470798579	-25.15342083695950	4.98664871368940
H	35.55096974493848	-24.89559423994252	4.11544817247645

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B3LYP Scan/Hydroxide IPC Model/Triplet/210 degrees Constrained Optimization

C	30.42724496631860	-24.85480175770702	2.51420620422786
C	35.82856181066688	-24.59021790939882	10.87120702836224

C	39.54440265145662	-29.58340429978611	5.89258824194242
C	33.80648158498287	-28.51027748966304	0.46408988520301
N	33.18430250181244	-25.55794491539589	4.96310621279119
N	34.71682917564950	-25.51489922226637	7.40976118932551
N	34.96764493537518	-27.47985036419493	3.88070741320230
C	32.90597285754360	-26.70044125117963	2.81990491267245
C	32.86587063186443	-24.01419096733228	6.84034795376961
C	36.57053461213596	-26.56717060941641	8.60141058776918
C	37.11518770164867	-28.59299432638611	4.25560073654982
C	30.46438442753657	-22.98147039551912	5.17430632310804
C	33.40166216749432	-22.80177918405162	9.64502153404253
C	39.11724842843135	-28.31422016272391	8.86187472288226
C	36.69119658411037	-29.69093829219640	1.38865712950399
C	32.51445594884714	-25.78553730402176	3.79415374448098
C	33.87304986785430	-24.47811668982850	7.68387262182810
C	37.04999894640580	-27.35883450628334	7.56288721427085
C	36.00346577585955	-28.27353192524302	3.48265155435962
C	31.38136948591454	-24.88083991315097	3.67226042143234
C	34.13525065742588	-23.95033352680284	9.01725578909729
C	38.26826976595825	-28.15826097681921	7.63485312787670
C	35.76314675980793	-28.78235999284809	2.13981661843319
C	31.39900325198916	-24.09074491682999	4.79152252579081
C	35.15377437243056	-24.70375008999771	9.53600548423956
C	38.44874296409608	-28.68736385787306	6.38785312173908
C	34.54705884552018	-28.28758746119912	1.74982931601916
C	32.53098695622774	-24.53589323809384	5.59197265990926
C	35.51266677855531	-25.66769205586676	8.50472547436136
C	37.32487238155286	-28.22618724759417	5.57972981270066
C	34.07146466114877	-27.46213853725178	2.85041979537801
N	36.50108003170399	-27.43421489572786	6.31899948758321
Fe	34.82465738644497	-26.53400257497747	5.65892063509775
C	32.67654046703059	-31.53369245111472	5.93453793225596
C	33.02349563985811	-32.32389861096289	7.19305001663827
C	32.45190212692332	-27.67815457732504	7.29717329401921
C	33.62171068854001	-28.00165377501233	6.39962700560336
C	33.79565308690105	-29.40654811958185	6.12132354637601
O	34.82703298446265	-30.02277824995505	5.88820156386217
O	32.58036884491511	-30.13719086067250	6.18878049493590
H	29.68886148623253	-22.82721829229560	4.41574846964403
H	30.99399046294669	-22.02656530832263	5.29936919635409
H	29.95390019638151	-23.18749658014577	6.12545190079951
H	30.93664368512820	-24.62184050199829	1.56826975007292
H	29.92901183181547	-25.82428427382726	2.37489862365325
H	29.64336768968904	-24.10243125485232	2.65504745346779
H	33.53994612086505	-27.56209820236389	-0.02293159274746
H	34.40601019343273	-29.08609211453007	-0.24982249144159
H	32.86856208289371	-29.06144171832635	0.62224349785889
H	36.32739077145786	-29.88771959747878	0.37395902086844
H	37.69839176435066	-29.26113593596071	1.29893982439118
H	36.80250071265373	-30.66180635934795	1.89105286778949
H	33.78383717608966	-22.58178860221744	10.64806311745807
H	32.32613049946644	-23.00683220456115	9.74224008152172
H	33.49714235188753	-21.88361195307319	9.04868541009724
H	36.89500942241254	-24.34432520391160	10.76945797805162
H	35.77320655229392	-25.53057791019958	11.43732370009090
H	39.96976496406861	-28.97767691158560	8.67903794961817
H	39.51936505179106	-27.35131951576351	9.20802594454779
H	38.54598987302305	-28.73900403192280	9.69921523594605
H	39.15071240493722	-30.55062493498836	5.55132563855962
H	40.08075063537390	-29.13788510061447	5.04293848312356
H	40.28392949687702	-29.78845036550389	6.67488142880366
H	35.37031037386522	-23.81026402562859	11.48929097223736
H	32.30173724588014	-32.11838730506672	7.98968397412509
H	33.01674593172671	-33.40248823026540	6.99161176434610
H	34.01790350403645	-32.04483363138529	7.54554778128918
H	33.42640254330671	-31.71547226295874	5.16005716141588
H	31.69262958230533	-31.82847553383986	5.55364856170066
H	32.28944925040868	-26.60733362514355	7.40076389274700

H	31.52139898405250	-28.13327285480506	6.93441414384294
H	32.60750714084858	-28.08174116665248	8.31140781435169
H	32.283742531666579	-26.78027226352993	1.93340091482979
H	37.11539823082745	-26.59502537637684	9.54057973985118
H	37.85954669890568	-29.24010004204010	3.80112314492984
H	32.25901613481638	-23.19124339813469	7.20690685687956
O	35.89103161144005	-25.15395076987173	4.99460656438893
H	35.53013024944457	-24.89058868125807	4.13462123289449

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B3LYP Scan/Hydroxide IPC Model/Triplet/220 degrees Constrained Optimization

C	30.40206759748441	-24.91231406705655	2.56502245687493
C	35.89187075893097	-24.50752075926254	10.86034499067400
C	39.56002057165598	-29.57850269156904	5.91961436606290
C	33.76884006989613	-28.58548096385394	0.53307456892686
N	33.18664496464883	-25.56908088582710	4.99582300670877
N	34.74479440160950	-25.48563391681665	7.42536005510086
N	34.97018284363460	-27.49674434058546	3.91807212993713
C	32.89517758512158	-26.73731815533586	2.86799686262698
C	32.87226152343228	-24.01004915044837	6.86091650698815
C	36.62338491833842	-26.50566009947954	8.60581201496878
C	37.11792441944770	-28.60996948047224	4.29087259870382
C	30.44921950706687	-23.01050052156896	5.20429974468136
C	33.42681133281211	-22.76268461022465	9.64659252377126
C	39.17003975308354	-28.25238055813248	8.86868607877066
C	36.65854795517349	-29.76035849480931	1.44754728090522
C	32.50799604471820	-25.81359255349652	3.83557194817977
C	33.89241992639563	-24.45590737981887	7.69864869975043
C	37.09439735794302	-27.31009960862565	7.57346928016050
C	35.99922400078655	-28.30149282768322	3.52301444513792
C	31.36722390514803	-24.91842837669403	3.71423817123826
C	34.16529147469797	-23.91020564148325	9.02273973167093
C	38.31057787702632	-28.11242596597867	7.64708372542965
C	35.74223099733884	-28.83489226097625	2.19276783235933
C	31.38865676489090	-24.11692776988899	4.82518295574253
C	35.19970231625177	-24.64531909221938	9.53636304048835
C	38.47546697550236	-28.665741915665965	6.40870998371597
C	34.52373819224321	-28.34234784476750	1.80684508993856
C	32.53111986685280	-24.54564918783848	5.62015200371117
C	35.55609271386124	-25.61711195742976	8.51158674664960
C	37.34511865142980	-28.21441454983815	5.60405035335026
C	34.06238312194286	-27.49606325703120	2.89725691025764
N	36.53316555446932	-27.40397693436725	6.33638112177229
Fe	34.84465273592537	-26.52122437948263	5.68594014321046
C	32.73375672669905	-31.47310903184462	5.66207956246145
C	32.77413638650465	-32.35039873950871	6.90938029982874
C	32.47691329373908	-27.68494435792310	7.33596186104762
C	33.66297527528160	-27.99713444921059	6.45652913072408
C	33.85606585199601	-29.40126175239682	6.17784941419877
O	34.89842860907756	-30.03707877651216	6.12257747099186
O	32.63332774544008	-30.09024432614987	5.98420404143647
H	29.66539678406611	-22.87093078779837	4.45143136074809
H	30.97267186870053	-22.05026353638115	5.31335454079557
H	29.94933566041725	-23.20947920366141	6.16254005184033
H	30.90134889509622	-24.69024678841332	1.61114298561173
H	29.90683313807523	-25.88577399304308	2.44384046341343
H	29.61622246303630	-24.16147579201750	2.70303430440253
H	33.50176290951869	-27.64523615338831	0.03125193415704
H	34.35824109757933	-29.17738842643725	-0.17607152277536
H	32.82996625595566	-29.12885696617597	0.71103242303053
H	36.28272215756596	-29.97302163129723	0.44044188047347
H	37.66643896068808	-29.33661887640260	1.33920313967119
H	36.77178758205010	-30.72318227894332	1.96484922959093
H	33.81716240072061	-22.52879343728516	10.64332673257421
H	32.35444867346639	-22.97736441795891	9.75704496027453
H	33.50701158959794	-21.84968836424081	9.04012676069232
H	36.95268067851268	-24.24583536965859	10.74047769245006
H	35.85987683106156	-25.44268027719115	11.43677299577410

H	40.02118960017912	-28.91780034508699	8.68679713086428
H	39.57453146488130	-27.28511202173673	9.19946757238327
H	38.60596317251701	-28.66719035616437	9.71581490045381
H	39.15634405017840	-30.55034291211794	5.60405590149755
H	40.08890397625989	-29.15456239558640	5.05440707708642
H	40.30753698373146	-29.77150475230826	6.69736826629122
H	35.43024814411541	-23.72852298577611	11.47711416287981
H	31.90711767416626	-32.15529773877638	7.54814524302713
H	32.77200209316350	-33.41394189103433	6.63949241722743
H	33.68009355037766	-32.14158307533344	7.48162313246428
H	33.62661684082501	-31.64344068977694	5.05514531425077
H	31.84633055493100	-31.69733094537456	5.06039377628618
H	32.25020284808463	-26.62050370095627	7.36924126305327
H	31.57477151551928	-28.21806095601994	7.01014571391441
H	32.66286038600623	-28.00409741647798	8.37572712402677
H	32.26354120650718	-26.83190920410986	1.98966575955896
H	37.17858522467643	-26.51860497518370	9.53923005354559
H	37.85403101219368	-29.27054270432529	3.84240993384716
H	32.26145086345609	-23.18903243073459	7.22531090363536
O	35.88348261825374	-25.13662432248886	4.99108568409077
H	35.51234685836869	-24.89454979106868	4.12923892973648

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B3LYP Scan/Hydroxide IPC Model/Triplet/230 degrees Constrained Optimization

C	30.39642162165232	-24.97280541321263	2.57398456866314
C	35.94506492622786	-24.42373419863371	10.82752560663596
C	39.56979513713662	-29.59420146404016	5.95445936642678
C	33.80137618814344	-28.60460366049410	0.54274612133956
N	33.18352743722392	-25.60169760376247	5.01004020930667
N	34.76051465834359	-25.47596400347357	7.42701884831027
N	34.98328641217639	-27.51976962967077	3.93609938506395
C	32.91061142456986	-26.76575113274908	2.87732396850959
C	32.84878876300666	-24.04710597243320	6.87499141964178
C	36.66384658790428	-26.45838501501870	8.60076420679687
C	37.12909333267385	-28.63427435704201	4.31818537190285
C	30.40413686933962	-23.08843149222034	5.22585091029684
C	33.42363474607022	-22.74935657721922	9.63230601949237
C	39.20582510236466	-28.20919164645444	8.87971115853565
C	36.68354675972051	-29.78464213401720	1.47474617134408
C	32.51068544218090	-25.85050169654729	3.84726729368583
C	33.89113727605206	-24.46090959894198	7.70122637162701
C	37.12441676175363	-27.28427766263564	7.58090539170721
C	36.01371118917238	-28.32540557030966	3.54618583372621
C	31.35646843162738	-24.97236815212931	3.72748831550581
C	34.17339774620431	-23.89202946826460	9.01293179340720
C	38.33831478600236	-28.08925949630343	7.66157244581253
C	35.76376078728619	-28.85846481635106	2.21474183573742
C	31.36091016769699	-24.17889470498171	4.84398311010557
C	35.23139467753677	-24.59846784186247	9.51934318214485
C	38.49194319017987	-28.66820697032265	6.43340956236993
C	34.54834377959219	-28.36415885123495	1.82170970742706
C	32.50959639589962	-24.59300589439145	5.63845539014476
C	35.58941454687356	-25.57836265116733	8.50306325079972
C	37.35826218685384	-28.22736678617746	5.62748460793523
C	34.08090570335526	-27.51926979336339	2.91056867759772
N	36.55240227803296	-27.40165510948246	6.34999014320877
Fe	34.85723584043576	-26.52899209033627	5.69596034100504
C	32.54696470083900	-31.35610273640476	5.48623827146545
C	32.55336236527290	-32.30344178959484	6.68194916777017
C	32.68602101970320	-27.71830854383636	7.58161594416720
C	33.69416576845595	-28.00809367142731	6.49865625059484
C	33.80368981150659	-29.39730963979113	6.11634820295894
O	34.80456023832887	-30.08890324391320	6.00925989443001
O	32.53970211380221	-29.98840589306783	5.88453724256788
H	29.61706363927229	-22.96080949626079	4.47420509930976
H	30.91220003609612	-22.11990046795491	5.33503834508802
H	29.90909287605601	-23.29641005238868	6.18462699515579
H	30.89954591623427	-24.74961440749604	1.62242632333818

H	29.90634794636154	-25.94872028887279	2.45150887694351
H	29.60673879957057	-24.22514389328524	2.70713878859811
H	33.53885864385176	-27.66326694740520	0.04054938761857
H	34.39476359933740	-29.19614384809562	-0.16339553403896
H	32.86074922527612	-29.14714086595990	0.71366826726766
H	36.31433860166802	-29.99541849686093	0.46481585529243
H	37.69287633595610	-29.36251559115420	1.37394982855298
H	36.79113634539983	-30.74815591927697	1.99189800661584
H	33.81354502070214	-22.50585771159976	10.62691226548193
H	32.35405870544425	-22.97530146691049	9.74633670115454
H	33.49238662014940	-21.83854208767918	9.02105520093940
H	36.98872187664141	-24.10941680770700	10.68451002883298
H	35.97227469922285	-25.35783362375645	11.40566243819787
H	40.05438710751361	-28.87944161303206	8.70372887701161
H	39.61444628322514	-27.23705531508237	9.19044685445431
H	38.64700739442575	-28.60769983556650	9.73811095491494
H	39.15893096697840	-30.56618875140764	5.64896919814369
H	40.10203802949411	-29.18348851596625	5.08488825053089
H	40.31579737695750	-29.78445097184699	6.73436916376734
H	35.45882023313252	-23.66736320615563	11.45349569418911
H	31.71106221336955	-32.09224478475205	7.34810409404042
H	32.47970645066471	-33.34775226661191	6.35348746460670
H	33.48032843689087	-32.18370621811933	7.24567730713983
H	33.41637103043083	-31.54718143372925	4.85194522345715
H	31.63692231348950	-31.48961024498724	4.89179120155609
H	32.20193585842917	-26.74583319230478	7.45450006349906
H	31.90234829980764	-28.48239413691515	7.64730158693467
H	33.18769577377256	-27.67924630571920	8.56209581229346
H	32.28345098404245	-26.86233701136661	1.99605314706309
H	37.22953683287580	-26.45073720881559	9.52792541093159
H	37.86352513948039	-29.30030519789779	3.87518382247747
H	32.22421307747665	-23.23713451417099	7.24083689838837
O	35.88081546980872	-25.14174460661968	4.98388993412803
H	35.48063382229471	-24.88339926598836	4.13994594795481

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B3LYP Scan/Hydroxide IPC Model/Triplet/240 degrees Constrained Optimization

C	30.38353893740155	-24.98735879556161	2.59886154437824
C	35.98685375631036	-24.37397725532137	10.81209304033860
C	39.55460054032267	-29.61868833073599	5.97446496121388
C	33.76818012780725	-28.64228773722265	0.57827238457203
N	33.18002496706479	-25.60416419890858	5.02731676191413
N	34.77208484495620	-25.46045142524936	7.43290730387869
N	34.97148262055485	-27.53567998484647	3.95684093512351
C	32.89741649238872	-26.78002311542732	2.90196122733621
C	32.85176022239209	-24.04127378358037	6.88615099289322
C	36.68748211892374	-26.42912511146591	8.59868108088079
C	37.11236815484132	-28.65972961776572	4.33993669536599
C	30.39863182528910	-23.09324848405569	5.24367041585141
C	33.44797878922348	-22.71881331591492	9.62746619749166
C	39.21983294881800	-28.19243781471939	8.88307659114760
C	36.64652705768363	-29.83317637416920	1.50808793461743
C	32.50266924003227	-25.85909712377341	3.86860439716012
C	33.90202017848177	-24.44588075083132	7.70694138352818
C	37.13840784641393	-27.26712823204526	7.58453929500914
C	35.99526578526042	-28.35152802432291	3.56965011382385
C	31.34721017814401	-24.98218557245653	3.74929682463297
C	34.19493316427245	-23.86493595119664	9.01100913900291
C	38.34694251159372	-28.07986629044522	7.66807005016843
C	35.73558460884966	-28.89533192383128	2.24450844306341
C	31.35456182779944	-24.18477332960716	4.86279434496761
C	35.26029778607274	-24.56340296250170	9.51302784264376
C	38.48823788808376	-28.67630469623798	6.44697871707837
C	34.52177883497373	-28.39588271639250	1.85221959592555
C	32.50693562520864	-24.59446185364972	5.65443839667310
C	35.61129352083021	-25.55121830877071	8.50199509939375
C	37.35313059627956	-28.23671878275089	5.64220423493413
C	34.06438670307882	-27.53867894884218	2.93546605292801

N	36.55834230955664	-27.39473794887085	6.35836863875280
Fe	34.85990249572137	-26.52402476876550	5.70831173642842
C	32.60813285696663	-31.30521788701027	5.33210330388611
C	32.47134867765805	-32.26960775734485	6.50552869250944
C	32.72868901545633	-27.74523256571545	7.64466328195209
C	33.70714135582964	-28.00385996745810	6.52794750903459
C	33.82926077229825	-29.39423544595150	6.14125486550989
O	34.81408033453992	-30.11396585470495	6.15696764642111
O	32.59041061412903	-29.94044750411877	5.74698946887964
H	29.60833794867475	-22.96954003090342	4.49475409360499
H	30.90654272359606	-22.12389855800100	5.34627430302479
H	29.90780969183487	-23.29713480090848	6.20549156620197
H	30.88410614684535	-24.76969132763298	1.64467972851171
H	29.89178109927366	-25.96321302408483	2.48284191201856
H	29.59531890669853	-24.23789320531152	2.73058307568301
H	33.50976254173013	-27.70347849454455	0.06931259681560
H	34.35497307420121	-29.24346433246417	-0.12522752597300
H	32.82476215567244	-29.17717609192116	0.75752865917569
H	36.27090392267127	-30.05087876176706	0.50200286924188
H	37.65757070921619	-29.41746967084085	1.39827465342806
H	36.75200969478492	-30.79283572230335	2.03284912305293
H	33.84204896619255	-22.47029446449762	10.61919873487382
H	32.37886437379157	-22.94388555424359	9.74701990328284
H	33.51446969806337	-21.81108680871332	9.01132212597227
H	37.02532214098440	-24.04895301300508	10.65565262796679
H	36.03091876265590	-25.30450347149464	11.39488147294270
H	40.06599309687059	-28.86602293377733	8.70835002082715
H	39.63208386133703	-27.21895848956447	9.18459135422070
H	38.66399235829853	-28.58323398582113	9.74695614115813
H	39.13324814476628	-30.59231126138054	5.68904359068742
H	40.08271089600571	-29.22702716070313	5.09369255490549
H	40.30567100328354	-29.80186383851349	6.75120764567238
H	35.49945308188901	-23.61954433134455	11.43953378944326
H	31.56423314530434	-32.05680117870175	7.07984094896892
H	32.41913400460789	-33.30708917103374	6.15216142974094
H	33.33253885225319	-32.17528364696741	7.16923005499844
H	33.53261996548859	-31.50685357394138	4.78542386111085
H	31.76103550675166	-31.40761047611545	4.64594738539475
H	32.26962316590083	-26.75496711264840	7.57905746190467
H	31.92233754857871	-28.49004288808693	7.68023926546808
H	33.24319769121993	-27.77860724468470	8.61975430631743
H	32.26602701512792	-26.88039152153483	2.02414347073164
H	37.26026264886190	-26.41276394888277	9.52136245335949
H	37.83922851508496	-29.33692984190293	3.90140031356379
H	32.22758052388579	-23.23059301247476	7.25112627614292
O	35.87586334622222	-25.14308069379297	4.97426961697861
H	35.46284409286493	-24.88704938594970	4.13586033926947

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B3LYP Scan/Hydroxide IPC Model/Triplet/250 degrees Constrained Optimization

C	30.36018723006532	-24.98283360978265	2.62759092281780
C	36.00456223370276	-24.33613916768093	10.80954854579299
C	39.51552840115426	-29.64780237741051	5.99820153785990
C	33.70353619490663	-28.68290442877854	0.62587018846276
N	33.16533591111095	-25.59363072879032	5.04743314841125
N	34.77399439933701	-25.43368391022380	7.43942403512606
N	34.94300004086843	-27.54164293778497	3.97972446174993
C	32.86631332776978	-26.78463417180126	2.93221206834409
C	32.85059674091741	-24.01729184746256	6.89730195452408
C	36.69682522673770	-26.39595959492442	8.59821711178746
C	37.07365603914111	-28.68492482182390	4.36570434863585
C	30.39521029888561	-23.06980754900225	5.25859352414676
C	33.45624965717365	-22.68914834726407	9.63457778010985
C	39.21551307171119	-28.17731951824380	8.88803042006568
C	36.57619483130132	-29.89134300066957	1.55096036418945
C	32.48165585233686	-25.85408730968626	3.89374004988245
C	33.90376051337808	-24.41993759724387	7.71539141142353
C	37.13802720679767	-27.24452488800072	7.58887455861511

C	35.95480916036811	-28.37515272797978	3.59735923239142
C	31.32933345235994	-24.97318566516699	3.77338106548673
C	34.20270420468061	-23.83471111919019	9.01656062396992
C	38.33879910868667	-28.06812966098466	7.67553939489170
C	35.67949524533457	-28.93541511585098	2.28192697398435
C	31.34494373819052	-24.16790653874150	4.88111616660470
C	35.27223133097358	-24.52943571228299	9.51431914882086
C	38.46555335345863	-28.68332245633903	6.46244784306580
C	34.46851491717668	-28.42767207180293	1.89131793261916
C	32.49927712852892	-24.57654216839676	5.67021669869963
C	35.61946430067216	-25.51965040014296	8.50409498619887
C	37.33055957345230	-28.24183962866900	5.65865735293100
C	34.02789141192429	-27.55110165604290	2.96593312705311
N	36.55051091096259	-27.37981277998652	6.36730930076706
Fe	34.85026275865720	-26.50740070701799	5.72285607350817
C	32.95735625127902	-31.32405198843479	5.19683730292287
C	32.51105502243217	-32.26295096566466	6.31285935571826
C	32.63163635404389	-27.75012928142683	7.58095068970532
C	33.71403195284327	-27.99034345385191	6.56117604518721
C	33.93329357466270	-29.39363102863289	6.25266657903789
O	34.88503867182677	-30.10087383732228	6.53236081347970
O	32.84045838060257	-29.95013870649183	5.56941574841722
H	29.60172578971263	-22.94852432914907	4.51267238747102
H	30.90747345260970	-22.10179049092997	5.35152444350440
H	29.90830231735515	-23.26457800925160	6.22429633437523
H	30.85715248809942	-24.77497143105608	1.66936346570652
H	29.86336409829668	-25.95727954470473	2.52151856532570
H	29.57600808843823	-24.22875596361497	2.75715457952171
H	33.46171420855154	-27.74885564239653	0.100141110245194
H	34.27433610016504	-29.30924975032789	-0.06873600299285
H	32.75023992428585	-29.19437916605475	0.81999119921122
H	36.18764724780650	-30.12316034247420	0.55297222883282
H	37.58848796571036	-29.48402740308996	1.42246684890690
H	36.68270461775619	-30.84328214884851	2.08952486477780
H	33.85025185507590	-22.44246226459833	10.62680297119083
H	32.38704248488948	-22.91394924822240	9.75344775463456
H	33.52333483668798	-21.78031618275676	9.02003132190787
H	37.03925773320364	-24.00149199378672	10.64821898462633
H	36.05998954938771	-25.26758901117975	11.38977439077026
H	40.05870375996762	-28.85476763084634	8.71392268435666
H	39.63207029547565	-27.20381014531470	9.18333203460289
H	38.66091149066640	-28.56223686064287	9.75530099028765
H	39.07930961169176	-30.62228133770503	5.73899066122534
H	40.03838977973825	-29.28175161071303	5.10342023084491
H	40.27296919379226	-29.82341353150639	6.77047208198313
H	35.51400973461161	-23.58746165905769	11.44144341456770
H	31.49001302276772	-32.02997992665698	6.63055682075876
H	32.53677288202104	-33.30719660896698	5.97747386420673
H	33.17433439295988	-32.16150408893881	7.17373941722890
H	33.99161912380153	-31.53642163306530	4.91603224412535
H	32.31875911788517	-31.43667074796232	4.31509032689823
H	32.26273986395351	-26.72265619498101	7.56498816218950
H	31.76908124642251	-28.41897498081539	7.43690827530824
H	33.00131745906895	-27.93328504612068	8.60570975099032
H	32.22851685062722	-26.88940937638831	2.05954950781435
H	37.27487531974072	-26.37493136484244	9.51749511735168
H	37.78970057706633	-29.37722580359488	3.93286185569006
H	32.22937265604116	-23.20381467257210	7.26107225972676
O	35.85794237248850	-25.13563255681602	4.96382237688381
H	35.45709966376656	-24.91248136605553	4.11025293733078

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B3LYP Scan/Hydroxide IPC Model/Triplet/260 degrees Constrained Optimization

C	30.36676096646831	-24.85344183340094	2.61594031343177
C	35.99458079567787	-24.39506088361759	10.82142970783119
C	39.44088154194733	-29.70146423961327	5.95384773138250
C	33.60367425959099	-28.64878413342131	0.61760364006237
N	33.14977343926075	-25.54443248570645	5.03902962771735

N	34.76249999238228	-25.42802179575776	7.43125823170057
N	34.88635822403413	-27.52346994171340	3.96148774319362
C	32.82793372627909	-26.71640038904009	2.91644749562578
C	32.85634521992977	-23.98320906050713	6.90570103791435
C	36.68074273142594	-26.41671380809420	8.57477555343274
C	36.98334494298071	-28.72754724652587	4.34758678415398
C	30.43135657288010	-22.96629803736453	5.26589063509546
C	33.45423168136821	-22.71656861525302	9.67332541871418
C	39.19040661811954	-28.21221689695479	8.83866641751836
C	36.44268163239214	-29.93406359840905	1.54060597260226
C	32.46469363960952	-25.78013008515073	3.88125522700820
C	33.89850997335579	-24.41394450446227	7.72320876985366
C	37.10627018970795	-27.26708092772397	7.56088361142802
C	35.86937659686771	-28.39093552019013	3.58208722508740
C	31.33248004008970	-24.87346098155700	3.76443121194940
C	34.19855200619102	-23.85233155628316	9.03518474474615
C	38.29949395238175	-28.10161707123572	7.63686060119591
C	35.57463818744063	-28.95086734397340	2.27004220458124
C	31.36110022298498	-24.07846004089498	4.87963859743755
C	35.26471522001978	-24.55949312617989	9.52100151290970
C	38.40426948949450	-28.72655019661740	6.42649830100138
C	34.37939399183858	-28.40874404948001	1.87933995215762
C	32.50339022555444	-24.51811262905824	5.66853858422688
C	35.60722702907930	-25.53508157955872	8.49435902793306
C	37.26467267183787	-28.27733883679797	5.63404296332228
C	33.96814720996671	-27.51328128885561	2.95080387203414
N	36.50457965671503	-27.40007556403166	6.34602261100493
Fe	34.81811773378929	-26.49222386018375	5.70872218258594
C	33.55490077560837	-31.46209728440342	5.40081670074642
C	32.73949337887685	-32.30787335800355	6.37256559028329
C	32.39992863923680	-27.71783858341470	7.32906730769408
C	33.66858352674731	-27.96521723122398	6.55590233287362
C	34.03237016803038	-29.37529990823814	6.49762708105296
O	34.85452339607258	-29.97548869128262	7.16580830063637
O	33.27580686397412	-30.06749445902991	5.54695405074440
H	29.64359051703136	-22.82115052078998	4.51825842992186
H	30.96173561883294	-22.00958488843360	5.37229561424089
H	29.93644578261983	-23.16290407624405	6.22716260218596
H	30.86876444629893	-24.63682797284125	1.66225627166818
H	29.85842696316770	-25.82003545296070	2.49346385505335
H	29.59104303679110	-24.09233201666795	2.75499039732076
H	33.38013048949691	-27.71037268628287	0.09154485384381
H	34.15782765470605	-29.28826514555529	-0.07849905596401
H	32.64022361032153	-29.13881693217989	0.81671600113440
H	36.04348677598872	-30.16138365394470	0.54576720458808
H	37.46458913304090	-29.55376313259624	1.40460181788398
H	36.52781296110616	-30.88572566737292	2.08350771832748
H	33.85437967704263	-22.48236789617883	10.66611422273028
H	32.38623460865736	-22.94520568736048	9.79626775973731
H	33.51537115899814	-21.79950913635400	9.07054293653232
H	37.03678731554808	-24.08065802280866	10.66815323119467
H	36.02764606653493	-25.33376510154626	11.39158315122264
H	40.02678134090707	-28.89619222048346	8.65721277092174
H	39.61730130150310	-27.24044577792513	9.12459433227059
H	38.64314011706111	-28.59004370803771	9.71344901603705
H	38.99477590149187	-30.67322241752454	5.70074883360994
H	39.95845073780038	-29.34186721103839	5.05333944676435
H	40.20389800817924	-29.88214765178647	6.71929440835882
H	35.51667835414251	-23.64300838678532	11.45896623149161
H	31.67039174285733	-32.10223852035691	6.26194050280595
H	32.90393682516201	-33.37769852050657	6.19404432133646
H	33.03053760139579	-32.08233190537162	7.40033132641142
H	34.62319471000141	-31.63421844828451	5.55018717454592
H	33.29730089991154	-31.69866741543437	4.36400377906055
H	32.06626755737544	-26.68193797721538	7.25902321568011
H	31.57151641476984	-28.35610609329592	6.97677434076472
H	32.52525790735069	-27.94344785451795	8.40370590982629
H	32.18843534217593	-26.80256303442700	2.04292239588289

H	37.26426878332163	-26.40566953650233	9.49069886803293
H	37.68133500794759	-29.43694707958866	3.91261497650323
H	32.24543354776548	-23.16628838682600	7.27900033574026
O	35.84707438949741	-25.13695947514273	4.95375065809986
H	35.49762971599043	-24.95818228863056	4.06771061136219

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B3LYP Scan/Hydroxide IPC Model/Triplet/270 degrees Constrained Optimization

C	30.32591412739604	-24.91471003751922	2.66161098253356
C	36.05322665525582	-24.29836200239031	10.78895362231658
C	39.40809301952918	-29.74340590707948	6.01256658715787
C	33.57063080706573	-28.70567190128106	0.67313406913399
N	33.12833002498577	-25.57029334568518	5.07241347590006
N	34.77096589462253	-25.40569181283749	7.44072945690199
N	34.86654918974497	-27.55078689218662	4.00188676798363
C	32.79842493878738	-26.76209197270995	2.96236819446489
C	32.85464697740552	-23.97553286987498	6.91365687301489
C	36.69803572886734	-26.37832376824121	8.58416055152856
C	36.95838569113159	-28.76285213808081	4.39538039789167
C	30.40632016402231	-22.99496216942437	5.28716802058522
C	33.49835495722751	-22.64215901416680	9.63994775594279
C	39.18866286756229	-28.19826766091699	8.87030638416490
C	36.41423280670417	-29.98305963230165	1.59691822019813
C	32.43565420955738	-25.82083144829631	3.92224905804111
C	33.91204662961334	-24.38448251707544	7.72296558566297
C	37.10784020566101	-27.25445244525930	7.58582844886527
C	35.84637710105152	-28.42405390721466	3.62794973644811
C	31.29942733134635	-24.91938489551717	3.80367268509174
C	34.23163960517988	-23.79380801760261	9.01749428135619
C	38.29295553677485	-28.09953821124475	7.67094717211450
C	35.54692812387296	-28.99572955048742	2.32192097317260
C	31.33467768170423	-24.11093615401505	4.90876817414956
C	35.30343177169659	-24.49204927332840	9.50386065297080
C	38.38476303154398	-28.74820317939401	6.47173029086820
C	34.35031814527104	-28.45683843325658	1.93084258699566
C	32.48538951072725	-24.53680137393758	5.69315231667531
C	35.62925054576106	-25.49166545977495	8.49481974298627
C	37.24628017558596	-28.30123759868868	5.67658347644254
C	33.94341719669108	-27.55195331086755	2.99608692995019
N	36.49714600491443	-27.40538509547051	6.37709980303353
Fe	34.80698805861249	-26.50083219101968	5.73558074505371
C	33.66371592299335	-31.35635625686632	5.18746469394880
C	32.74439548475299	-32.27458266521199	5.98502678859170
C	32.45556144822149	-27.71073743863871	7.47373024761028
C	33.68021289927522	-27.96357439932141	6.63453952279356
C	34.00141231990995	-29.38271073653924	6.51557209192473
O	34.71653645187624	-30.05275047230409	7.23969368897024
O	33.37061705395209	-29.97646275741292	5.42466421299301
H	29.60839548267424	-22.86582230965647	4.54739959323965
H	30.93476983708497	-22.03475166732681	5.36923602525026
H	29.92477008025989	-23.17578031615086	6.25821776437201
H	30.82155105041231	-24.71034189419979	1.70191610008521
H	29.81698590855517	-25.88286038380578	2.55492286446593
H	29.55105671539364	-24.15186983929802	2.79587580582880
H	33.36046809567873	-27.77267257067507	0.13193922034106
H	34.11510842727041	-29.36424575855002	-0.01269791069517
H	32.60029503750568	-29.17819233294922	0.88043280143993
H	36.00663741626966	-30.22612694991408	0.60924458585600
H	37.43220336860347	-29.59795487962236	1.44558884610061
H	36.51123086298531	-30.92672135748576	2.15156055083565
H	33.91046524660064	-22.38894036541646	10.62312968432894
H	32.43105718590910	-22.86429141678760	9.77942030452263
H	33.55596172785005	-21.73805883831592	9.01753172865969
H	37.08982302167778	-23.97728913736939	10.61292034136165
H	36.10440132354918	-25.22634635422711	11.37501729710860
H	40.02144394638766	-28.88793600979071	8.69407370528558
H	39.62060619660274	-27.22459467577281	9.14163173864510
H	38.64394375606432	-28.56243729754251	9.75246867405214

H	38.95045217311670	-30.71581885222000	5.78356350126506
H	39.92255532614124	-29.40855485600807	5.10085489824402
H	40.17494469051556	-29.91539916863679	6.77616978315643
H	35.57895047440589	-23.53935340960007	11.42096571945808
H	31.69478313312454	-32.04358848484551	5.77891891255929
H	32.92176096829972	-33.32610611768695	5.72785257697080
H	32.92335569992662	-32.14657010381301	7.05422345116109
H	34.70908693196522	-31.55150008353625	5.43726317119176
H	33.52261071228698	-31.49581396559567	4.11172789157644
H	32.25998026258463	-26.64700913218959	7.61342691996408
H	31.54687919690777	-28.15149472694469	7.02457823178441
H	32.54704233760960	-28.16026446247363	8.47867359354387
H	32.15371786607028	-26.85931152333441	2.09386824703980
H	37.28998911094193	-26.35141184119328	9.49432129308253
H	37.65020507630357	-29.48173101671764	3.96613173767520
H	32.24688004454180	-23.15247612115829	7.27854199386159
O	35.82579772771091	-25.15583530951276	4.95034098510711
H	35.47698643635618	-25.00058109923463	4.05960144684488

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B3LYP Scan/Hydroxide IPC Model/Triplet/280 degrees Constrained Optimization

C	30.30635889549349	-24.84875642156879	2.65903012196607
C	36.03956505946908	-24.34765948380891	10.78825388356763
C	39.33367039995164	-29.80060147683486	5.98200311324473
C	33.49759136222251	-28.67962167534915	0.65703633416961
N	33.10519807413112	-25.54602889249551	5.06161253657733
N	34.75401689179542	-25.40840773097320	7.42645689765868
N	34.81834999653203	-27.54097637641674	3.98199206529190
C	32.75123124138853	-26.73482038502298	2.95404992433553
C	32.86525134015282	-23.94276551315263	6.90031176750102
C	36.65437919302649	-26.42639600966152	8.57453125046260
C	36.89982663404059	-28.77453709034828	4.36355127751044
C	30.43219324153191	-22.92044629432409	5.27679013379092
C	33.52479943788016	-22.63220962795615	9.63442672549036
C	39.11142048815411	-28.29146356932520	8.85878429770958
C	36.34184347526629	-29.97064163637768	1.55872013867785
C	32.40470067564185	-25.78760481036499	3.91448706192173
C	33.91394202032858	-24.37240815779856	7.71011580843800
C	37.05324973717570	-27.30372793543881	7.57260815710084
C	35.79101793152248	-28.41825946155790	3.59978781769901
C	31.28364859463266	-24.86731933606400	3.79769249752423
C	34.23983554629365	-23.79369670830316	9.00901048206873
C	38.22570197083825	-28.16574860790296	7.65463774371668
C	35.48289024774967	-28.98210787807795	2.29214511571941
C	31.33808431431917	-24.05527061286573	4.89961168515990
C	35.29437158329866	-24.51616841047323	9.49702720050776
C	38.31679320741260	-28.80158327504952	6.44790522210309
C	34.28638113172856	-28.43734687987404	1.91017235103596
C	32.48361861642946	-24.49888392171823	5.68115731804840
C	35.60474517304968	-25.51743182020495	8.48420736933081
C	37.18828430318649	-28.33208212278244	5.65193281996716
C	33.89010351931816	-27.53378997309740	2.98086202722215
N	36.44651376994179	-27.43498054368337	6.35933040034187
Fe	34.77006837500311	-26.50060461391137	5.71938837217043
C	34.04976101344952	-31.37761597312065	5.36806967666266
C	33.04896210746212	-32.32459680952445	6.02110242804395
C	32.36437217202251	-27.65656862645650	7.41012524073180
C	33.62643013384216	-27.93821007034395	6.63733216754821
C	33.99224156460046	-29.35049868311984	6.65056125787860
O	34.55873647235776	-29.95873981291048	7.54402409899557
O	33.64340021026274	-30.01039612163483	5.47892011326596
H	29.62607405110119	-22.78848053695417	4.54654330431042
H	30.97612830573877	-21.96738262708293	5.33911876557116
H	29.96180970060095	-23.08190656147775	6.25657148697273
H	30.79957621322119	-24.64013144224951	1.69893248896324
H	29.79164208288330	-25.81322083641112	2.54723959658588
H	29.53612232405805	-24.08271794007482	2.80145950993337
H	33.29434523100311	-27.74553546589440	0.11495522348910

H	34.03131578512025	-29.34540453854545	-0.03024313709754
H	32.52341965009187	-29.14136064324246	0.87055404997528
H	35.92469836213979	-30.21285293106634	0.57482940397147
H	37.35913972995086	-29.58738994152099	1.39805331610759
H	36.44265256320283	-30.91467470588071	2.11214676594660
H	33.94938107719165	-22.37973157856828	10.61247524752887
H	32.45661012504326	-22.84269729467916	9.78532995052852
H	33.58557390948395	-21.73128636884671	9.00785723626825
H	37.09073709819128	-24.07361026362886	10.61998714284961
H	36.04474490491953	-25.27369941928867	11.37973708517224
H	39.94038777702063	-28.98451351007173	8.67785384411838
H	39.54852332329171	-27.32582221531552	9.14956933264112
H	38.55615564291747	-28.66594420832106	9.72992600387007
H	38.87002940959357	-30.76587494712281	5.73527886706244
H	39.85797983642633	-29.45770694740157	5.07893485817794
H	40.09309351536579	-29.99050392175711	6.74870463733760
H	35.59293024359281	-23.56497926408044	11.41146134960336
H	32.04686910672331	-32.17154504309909	5.60873473719771
H	33.33390024508631	-33.37041566143195	5.85262420907770
H	33.01337409936691	-32.14640112127602	7.09719933112170
H	35.03851760728332	-31.49993045591168	5.81621378547631
H	34.11917573229363	-31.56376362909633	4.29249946493039
H	32.21613436893511	-26.59219580804329	7.59744961105103
H	31.46590696965239	-28.01349772727778	6.87345095715117
H	32.36091470817348	-28.16830823990575	8.38759522165403
H	32.10179712182124	-26.82457338419233	2.08821048767299
H	37.24143778076529	-26.41696658128718	9.48816625716572
H	37.58641970282629	-29.49399043717598	3.92674812524992
H	32.27299939900658	-23.10861649642428	7.26544785778775
O	35.80764849506219	-25.16662766041304	4.94016976701698
H	35.49319283094891	-25.03634983808707	4.03274829840162

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B3LYP Scan/Hydroxide IPC Model/Triplet/290 degrees Constrained Optimization

C	30.30332997763785	-24.71451229819025	2.65118687596107
C	36.01541299492381	-24.46443949940900	10.80402620537847
C	39.25372351748144	-29.85188423348255	5.89404128104380
C	33.35939786751005	-28.66026054824665	0.64717472820020
N	33.07996677911782	-25.50954626120819	5.04774614219221
N	34.72438120615092	-25.44244824968303	7.41958191636406
N	34.73149079472590	-27.54670992014678	3.96067633852641
C	32.67474849365759	-26.69523605469106	2.94816654974326
C	32.89624216161582	-23.90386835179973	6.89055650828072
C	36.58501716914856	-26.53084597656008	8.56632166443524
C	36.80888982763628	-28.79673306846220	4.30698092750987
C	30.516121374449787	-22.77828372598673	5.25847833798917
C	33.57205460313957	-22.64908471152623	9.64651599035054
C	39.03386362026281	-28.41276466501063	8.80762681831268
C	36.20178421534792	-29.97895080375424	1.50700666483737
C	32.36779391781222	-25.72897786202577	3.90395837424032
C	33.91859345050698	-24.38173265513468	7.70702590717051
C	36.96976040141824	-27.40107183350954	7.55173012333462
C	35.69323933042626	-28.42822372374129	3.56041237897003
C	31.28360076175954	-24.76572643128656	3.78614451068361
C	34.25324777303583	-23.82748399867183	9.01518927754901
C	38.14044125818646	-28.26591177798436	7.61137761420512
C	35.36469263339058	-28.98155908061294	2.25313914824905
C	31.37476332752808	-23.95019731808754	4.88352677602039
C	35.27703563193872	-24.59126003991962	9.504311921115104
C	38.22962828242326	-28.87347782922485	6.38839691288714
C	34.16780600931421	-28.42643368079045	1.88920085667968
C	32.50199749970680	-24.43672902925244	5.66508401262177
C	35.56177060619368	-25.59204018379730	8.48250670539943
C	37.09859214937909	-28.38859036517999	5.60646474120797
C	33.79425396357379	-27.52184941952437	2.96773266359719
N	36.35630654439751	-27.51101960609971	6.33894228550913
Fe	34.70733724711339	-26.52417290527904	5.70826380386414
C	34.67112120772499	-31.31930938095422	5.89960654188531

C	33.60130740333073	-32.38620245447266	6.09853872417142
C	32.08856468734006	-27.59363785501495	7.07526686381277
C	33.49663703433178	-27.90286203000286	6.63399358566353
C	33.88122431242678	-29.28298666415251	6.88635653715630
O	34.08439094775301	-29.79263970918100	7.98042684645793
O	34.09994969906648	-30.02003727460837	5.73281479871400
H	29.72392147515582	-22.60702539289535	4.52135346408267
H	31.10113651635444	-21.85084496994609	5.33146366660899
H	30.02915343186449	-22.92403150041968	6.23265852241348
H	30.79995650164247	-24.52992332597631	1.68798444562912
H	29.75100501047459	-25.65886503439635	2.54665342122097
H	29.56351107583968	-23.91903437413927	2.79327699513929
H	33.14895189868889	-27.72293611161292	0.11359600930912
H	33.88137733781063	-29.32307389857056	-0.05182439010920
H	32.38783814610836	-29.12196299651558	0.87295384217442
H	35.77721001449204	-30.20291805568317	0.52194000515206
H	37.22617683463459	-29.61477946887315	1.34730010612113
H	36.28471552810263	-30.93090024729031	2.05009394913389
H	34.00301939062038	-22.41440704772114	10.62619232815711
H	32.49803677302351	-22.82931501897692	9.79538517531073
H	33.65957357165446	-21.74694381046111	9.02485089652169
H	37.08241251778074	-24.25201212363769	10.64712272188598
H	35.96019698985777	-25.38870224356363	11.39569266211208
H	39.85841112692677	-29.10713916023705	8.61208590314534
H	39.47765840853371	-27.45298373981452	9.10731007295484
H	38.48296916818813	-28.79502127332646	9.67808886260029
H	38.79807931347062	-30.81215096946161	5.61494473970544
H	39.77754062332113	-29.47660794607482	5.00370466411669
H	40.01262501133397	-30.06044661846569	6.65629150259215
H	35.60777121381681	-23.65629862556908	11.42150707820591
H	32.87175626747457	-32.35735550631868	5.28328666380270
H	34.04933836061518	-33.38727761478302	6.12400282633575
H	33.07666510727677	-32.21809271600926	7.04116879682986
H	35.36002532904346	-31.30661969010503	6.74701930413699
H	35.23854209621211	-31.49958329639222	4.98204971882899
H	31.95617306494905	-26.54805600103210	7.36413558164321
H	31.36652176457172	-27.78208552055120	6.26178924957012
H	31.77899537439433	-28.21730821759118	7.92764512973596
H	32.01728432393828	-26.76849695460662	2.08674486355494
H	37.17079021018672	-26.54579719986566	9.48063087315895
H	37.49492438404813	-29.50419506577814	3.84997099711181
H	32.33438788892061	-23.04972786946778	7.25732970951766
O	35.79187388955578	-25.21450033869927	4.94702302641214
H	35.54390252918306	-25.12446212150487	4.01437709685009

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B3LYP Scan/Hydroxide IPC Model/Triplet/300 degrees Constrained Optimization

C	30.28863585600152	-24.73555937425454	2.65710503850298
C	36.00842115159895	-24.47544724738769	10.80204246865977
C	39.25230730004660	-29.85478922127138	5.88936936156975
C	33.36666201892901	-28.65780732206974	0.63609603874695
N	33.07496139027628	-25.52075376708245	5.04556513051867
N	34.72130811713880	-25.45175308307661	7.41573567203430
N	34.72642884024135	-27.55513598169287	3.95818260463145
C	32.66539065986188	-26.71082710230823	2.94937042918731
C	32.90355444235875	-23.90328559072251	6.87904991314947
C	36.56990166473788	-26.55216981588045	8.57036730679398
C	36.81253364366955	-28.79226863752935	4.29889671789938
C	30.51407089787930	-22.78696392403407	5.25450634715173
C	33.59174859407417	-22.63639659870309	9.62654338840300
C	39.01504571885668	-28.44018275553188	8.81332414184414
C	36.21853264287834	-29.95862331289426	1.49004773785223
C	32.35833397050808	-25.74490095551233	3.90546221904418
C	33.92532239460932	-24.38141789785317	7.69615832544243
C	36.95571643203305	-27.42112776859689	7.55490774795512
C	35.69585989655295	-28.42573679895503	3.55306791454278
C	31.27349563756709	-24.78206165267138	3.78830019362456
C	34.26298564298425	-23.82425525819497	9.00211453704462

C	38.12660737645955	-28.28603119812080	7.61426801770934
C	35.37281318265959	-28.97294267446939	2.24190466258271
C	31.37037496366174	-23.96102115182164	4.88106153651140
C	35.27666026470430	-24.59727933196869	9.49815365306342
C	38.22323382525317	-28.88314004079071	6.38669376589205
C	34.17125243592598	-28.42592719397965	1.88095097200162
C	32.50087040085209	-24.44438671216961	5.65999517983404
C	35.55437687363242	-25.60515637566901	8.48159585700092
C	37.09501763636946	-28.39416692810400	5.60294836689132
C	33.78973915124727	-27.53112884256058	2.96497069553509
N	36.34746985605833	-27.52424316808506	6.33876191416570
Fe	34.69991361892910	-26.53760980280600	5.70705770870869
C	34.69635339014584	-31.30597883072961	5.92032131081981
C	33.60799387189080	-32.36753599119216	6.03233030682382
C	32.12717781075094	-27.53065312496990	7.18072734741348
C	35.48592190673635	-27.90344337434554	6.64141868334757
C	33.82493878433208	-29.29356979547158	6.88089700403605
O	33.91583901012786	-29.83890685263809	7.97626062802952
O	34.15084756943607	-29.99961638710862	5.73426049139413
H	29.72556051926356	-22.61163300839493	4.51441014567168
H	31.10206652255302	-21.86180509217636	5.33143561348613
H	30.02265709321214	-22.93260188210755	6.22651156293729
H	30.78105314538630	-24.55142553685885	1.69162791762652
H	29.73857594899415	-25.68160360649611	2.55643702548702
H	29.54713257139048	-23.94192428859472	2.80063567013447
H	33.13894653062219	-27.71714218140068	0.11584977923937
H	33.90075662565537	-29.30096042915892	-0.07209326881392
H	32.40386875151096	-29.14074755577879	0.85512444656138
H	35.80295751188434	-30.17076906835564	0.49854243080127
H	37.24327651297428	-29.58993627267674	1.34393102712673
H	36.29900241149494	-30.91748492946861	2.02131659953016
H	34.03824833941182	-22.38726968905787	10.59563366976658
H	32.52016328431141	-22.81393266665664	9.79538828738960
H	33.66949279961227	-21.74412434905486	8.98978958508626
H	37.08584058655919	-24.32058201754986	10.65083650993120
H	35.90150756324414	-25.38075935950505	11.41594368535187
H	39.83381052322058	-29.14213167780515	8.62055079902203
H	39.46691247157208	-27.48436761767660	9.11390205491569
H	38.45827455920006	-28.81695400970603	9.68240390525420
H	38.80006513804163	-30.81221442196971	5.59557946174226
H	39.78271353425990	-29.46854056000551	5.00763370447289
H	40.00551611531419	-30.07119455997268	6.65507499802980
H	35.63608159469695	-23.63292934881514	11.39543479951845
H	32.93602172911882	-32.32357484144092	5.16977279665258
H	34.04711492317830	-33.37198301867303	6.07567418233791
H	33.02224823295681	-32.20616179795987	6.93911161762251
H	35.32784363107680	-31.31365254113573	6.81180994464535
H	35.32176691643883	-31.47852191709319	5.03972550906776
H	32.09434198649018	-26.51401095549625	7.58264115457915
H	31.36754782422154	-27.56663198362802	6.38247622979934
H	31.79917028228133	-28.21585177722723	7.97487622272602
H	32.00645207926242	-26.78585866058051	2.08923532583631
H	37.15181479998105	-26.57119138960705	9.48706534719411
H	37.50433249524962	-29.49148869625796	3.83789380920327
H	32.34655442513522	-23.04435751824877	7.24200466347919
O	35.78707505747044	-25.23026963377762	4.94418775752901
H	35.52952527377499	-25.13079283940672	4.01513303469913

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B3LYP Scan/Hydroxide IPC Model/Triplet/310 degrees Constrained Optimization

C	30.27810437349014	-24.74257900091641	2.65994296848024
C	36.00672420055942	-24.48424653469877	10.79827198947454
C	39.26050693585321	-29.83931510735773	5.87114255186593
C	33.34337809924817	-28.67940461787811	0.64399335049910
N	33.06905840781858	-25.52746792821766	5.04282785656980
N	34.71605249982929	-25.46154967589533	7.41387819659936
N	34.70994751535725	-27.57107116627215	3.96133577316695
C	32.6468687596514	-26.72814778849605	2.95550245799982

C	32.90930047247543	-23.90213582143534	6.87034529309204
C	36.56132584506764	-26.56574496987704	8.56992543673336
C	36.80654086274959	-28.79303289410965	4.29190468478641
C	30.52266210276122	-22.77984934348306	5.24500371056725
C	33.60135376505305	-22.63381727959993	9.61628349613501
C	39.01796955800037	-28.44066335258138	8.80184522212129
C	36.20492153834714	-29.96638324101258	1.48749056328293
C	31.34730401983568	-25.75489304144422	3.90675807417305
C	33.92679523196578	-24.38494351205262	7.69011201036489
C	36.94814932598995	-27.43159525855103	7.55208840260034
C	35.68288790722900	-28.43578545256734	3.55216325057762
C	31.26654582988319	-24.78761051944469	3.78809945738867
C	34.26616127732412	-23.82704789846760	8.99531450767924
C	38.12499414261429	-28.28897912733646	7.60575288401180
C	35.35718443892060	-28.98484405154068	2.24241224608189
C	31.37153156974853	-23.96064049411532	4.87573043974128
C	35.27428549465564	-24.60529073944851	9.49467260259410
C	38.22395797241235	-28.87893689785484	6.37488569110446
C	34.15123802219966	-28.44425370630943	1.88616539619103
C	32.50215970975911	-24.44538446902970	5.65369882494590
C	35.54773756232501	-25.61657316306188	8.48054878071129
C	37.09010472839846	-28.39545057704396	5.59580330429369
C	33.77015294867319	-27.55004855167534	2.97086279384341
N	36.33765804895459	-27.53449794078358	6.33695144487714
Fe	34.68794642709517	-26.55206951257532	5.70844012270733
C	34.77338297770934	-31.29229936975762	6.06331223457086
C	33.68312450363658	-32.35079944104186	5.93822642539232
C	32.11746785066277	-27.48945080023122	7.18912492849327
C	33.46298881999181	-27.90208001052561	6.64377101166142
C	33.76564191527543	-29.29277123653467	6.90984583148460
O	33.68364824543696	-29.85717045809374	7.99936528053501
O	34.26944249707596	-29.98048221212935	5.81874842628745
H	29.73059529304014	-22.60685518522971	4.50818660025597
H	31.11515482232264	-21.85672191724145	5.31122289225056
H	30.03639466998109	-22.91589410638997	6.22092947711224
H	30.76811975069887	-24.56604134610823	1.69183397471444
H	29.72327484981746	-25.68654606160094	2.56631587016988
H	29.54082458679022	-23.94469925730753	2.80161914488679
H	33.11818423020243	-27.74058091978327	0.11924331827691
H	33.87370814514959	-29.32823621723903	-0.06180909858829
H	32.37918009561365	-29.15749752815133	0.86727499179218
H	35.78460491046616	-30.18378844247057	0.49912191454460
H	37.22609415126703	-29.59084761569675	1.33393601934816
H	36.29529838117401	-30.92309747537595	2.02087715230173
H	34.04153791718259	-22.39138683504584	10.58992882041574
H	32.52664263162357	-22.80122746100562	9.77493956500861
H	33.69369180930273	-21.74082153066717	8.98242180128239
H	37.08247742362786	-24.31794355404037	10.64666642163604
H	35.90946211198717	-25.39440409461775	11.40642199471306
H	39.83897498212578	-29.13906721883919	8.60574583502925
H	39.46690797711474	-27.48328055297843	9.10181456820868
H	38.46599267035756	-28.82040778080864	9.67273316900149
H	38.81720145608620	-30.80106686952649	5.57775835737644
H	39.78274729646328	-29.44599927187352	4.98771255190510
H	40.01948685940997	-30.04915197823647	6.63297535145527
H	35.62707371946491	-23.64913800638439	11.39743034104124
H	33.18791563939676	-32.28056743710821	4.96495679735799
H	34.10526149397369	-33.35847318255820	6.03911524591077
H	32.93409918161173	-32.21074565312210	6.72016234951797
H	35.22823170916292	-31.33075903157926	7.05566784626568
H	35.55080915712801	-31.44152304350652	5.30799228471041
H	32.13115525322488	-26.49534637635044	7.64552487579734
H	31.37338012156251	-27.43854983004069	6.37848396373882
H	31.74491263180310	-28.19950667963617	7.93848039299013
H	31.98516963080289	-26.80537255864785	2.09767380371279
H	37.14433236705551	-26.58466521670394	9.48593728526634
H	37.50271208341860	-29.48507701214478	3.82649925301369
H	32.35783424800645	-23.03842701852358	7.23036293700411

O 35.77686206435189 -25.24714487970050 4.94084029496444
H 35.51139830988160 -25.14141723331081 4.01475305392479

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B3LYP Scan/Hydroxide IPC Model/Triplet/320 degrees Constrained Optimization

C 30.27771458514275 -24.73966660776492 2.66146823293746
C 36.00742067075566 -24.49669035629572 10.79946801031957
C 39.27904612679377 -29.81402696147757 5.85145830409081
C 33.33376464184678 -28.68638849013085 0.64542208268647
N 33.06725661426556 -25.53342477425061 5.04301953627612
N 34.70769930000152 -25.47926215588358 7.41982577886555
N 34.70033284864281 -27.58315995222103 3.96402021224394
C 32.63809684237569 -26.73689735472322 2.95905291594750
C 32.91402173684677 -23.90673587021699 6.86983521816215
C 36.55259933097334 -26.58488616616510 8.57464176542249
C 36.80519332875356 -28.79231805944336 4.28683893434277
C 30.53448363374556 -22.77338752069358 5.24266561484178
C 33.61379774269689 -22.635074516888347 9.61177345871796
C 39.02933483010708 -28.43436516676322 8.79007826167495
C 36.20181750248237 -29.96424877593656 1.48106116547378
C 32.34360349821683 -25.75981726981118 3.90803356054922
C 33.92638493636103 -24.39561374796200 7.69211880776399
C 36.94201877689299 -27.44526844277945 7.55296955536004
C 35.67690248304054 -28.44178989018327 3.55099769039703
C 31.26722366768407 -24.78752950840786 3.78855383485355
C 34.26951398900462 -23.83574699181777 8.99538720241313
C 38.12857416127525 -28.28997921362080 7.59884022770727
C 35.35131504644340 -28.98835344727627 2.24018405368273
C 31.37723143672743 -23.95897515357897 4.87456447531108
C 35.27243905831907 -24.61906074428147 9.49738504765922
C 38.23074904775191 -28.87117722776047 6.36414165574924
C 34.14243082535769 -28.45182258422992 1.88717067201642
C 32.50572520783126 -24.44812949499715 5.65283549379749
C 35.53952973204550 -25.63503247871807 8.48632045230224
C 37.08842723680075 -28.39699865329357 5.59134116011522
C 33.75988921782906 -27.56107314040366 2.97411230341718
N 36.32881023117351 -27.54885237295113 6.33960472380823
Fe 34.67706917050895 -26.57007477488448 5.71350324086422
C 34.80638888752556 -31.29493495184577 6.16163926614616
C 33.71740663260053 -32.33203992721384 5.90579994143162
C 32.10057461054510 -27.46676984608734 7.18208329075496
C 33.43375005947500 -27.91308955078475 6.63180780082407
C 33.69380248412415 -29.31098778379759 6.89921729880865
O 33.43525218177280 -29.91370435671628 7.94249151830703
O 34.36114191113690 -29.97004987185551 5.88115347465882
H 29.74301022841775 -22.59727183879251 4.50598165831613
H 31.13168186457704 -21.85319548462772 5.30749570461637
H 30.04797716568928 -22.90576890013950 6.21895756882573
H 30.76721316714490 -24.56542922626027 1.69268733145210
H 29.71940909481228 -25.68168414440906 2.56918064061589
H 29.54345695226571 -23.93909830636790 2.80363804636687
H 33.10750206759746 -27.74725844405570 0.12165008328444
H 33.86383764009458 -29.33432203238395 -0.06136209416579
H 32.37003859964000 -29.16515513579138 0.86921934759139
H 35.78083209251042 -30.18045246529068 0.49271595672332
H 37.22114815702392 -29.58396972536735 1.32690945970897
H 36.29695909509709 -30.92199915627830 2.01167010922590
H 34.05640330759733 -22.39174344660889 10.58409533835392
H 32.53799047589765 -22.79383198804847 9.77178120689228
H 33.71238216515307 -21.74549842286845 8.97407942101019
H 37.08408524765208 -24.33879850916377 10.64541139745300
H 35.90462404024996 -25.40277148612864 11.41280800514964
H 39.85391360161973 -29.12745590955250 8.59016128680453
H 39.47360827613863 -27.47356577456022 9.08616733334234
H 38.48541745768102 -28.81637799406523 9.66506096575094
H 38.84874378486271 -30.77977078134547 5.55182776826523
H 39.79414040149050 -29.40713139803666 4.96998576956280
H 40.04234055565205 -30.01889582837637 6.61033269029122

H	35.63472525332943	-23.65562492240960	11.39466060392963
H	33.33201201222612	-32.24071886983361	4.88565610090283
H	34.10886997694040	-33.34856386647736	6.03719792507780
H	32.89232588008518	-32.18525901466392	6.60472831590462
H	35.15032108413497	-31.35513986138169	7.19714905862054
H	35.65775458338581	-31.45165496131840	5.49261342884890
H	32.15921472876799	-26.50393075311312	7.69895796391796
H	31.37919394367084	-27.32388148223858	6.36345423408149
H	31.68003043308375	-28.20114165945887	7.87879850476647
H	31.97548712301407	-26.81333857631751	2.10184474281223
H	37.13776731495625	-26.60319880265324	9.48931748339152
H	37.50659214164171	-29.47595296561482	3.81684245843221
H	32.36776643161432	-23.03895146363548	7.22796011468581
O	35.77353732425578	-25.26589796448667	4.95267871431650
H	35.50386125715310	-25.14947782676938	4.02909845617178

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B3LYP Scan/Hydroxide IPC Model/Triplet/330 degrees Constrained Optimization

C	30.26420256620213	-24.76286040942380	2.67523623761696
C	36.011137731573499	-24.49078854785225	10.79849135750800
C	39.28780339263424	-29.80333038026158	5.85099148299722
C	33.31493610226141	-28.71932173244936	0.66741260738081
N	33.06460160598786	-25.54324131046952	5.04823731965205
N	34.71079390004024	-25.48048169907947	7.42151246982255
N	34.69083243114738	-27.59993576009858	3.97663545909338
C	32.62259278726665	-26.76271848113341	2.97641709716770
C	32.92361140877299	-23.90298476810606	6.86389767161111
C	36.55174556538665	-26.58798783859406	8.58043643371104
C	36.80535094484233	-28.7938207759141	4.29231950180483
C	30.54104310548134	-22.77429387854756	5.23738699832142
C	33.63015286206684	-22.62052624210113	9.59934476438454
C	39.03283054071317	-28.43268633712459	8.79311424412335
C	36.19512196050054	-29.97742050292682	1.49202420122423
C	32.33425950678289	-25.77774019971192	3.91921698589771
C	33.93509892058328	-24.39110622894407	7.68770735396849
C	36.94206558505166	-27.44741798199554	7.55814234081031
C	35.67089981133546	-28.45334811942925	3.56116592423165
C	31.25967995823727	-24.80366775999544	3.79733779497821
C	34.28010308685889	-23.82729687306021	8.98874497331161
C	38.13128790158549	-28.28893162308988	7.60240361475604
C	35.34168861418782	-29.00603447093757	2.25380477665118
C	31.37815351161584	-23.96574316186828	4.87531203427506
C	35.27778170981251	-24.61428054323374	9.49573265277257
C	38.23561084988500	-28.86611347861683	6.36617050707369
C	34.12749831861480	-28.47792788489703	1.90537343742250
C	32.50924038634945	-24.45150603633908	5.65206732946637
C	35.54108152543582	-25.63564623597541	8.48921725594003
C	37.09068496243364	-28.39481783166518	5.59500280784656
C	33.74581854406730	-27.58511444650031	2.99082250096063
N	36.32889018602818	-27.55064885642647	6.34516428911738
Fe	34.67220512933267	-26.58027676834665	5.72181588048810
C	34.81376076380137	-31.29104214565607	6.22311084928182
C	33.75734324016682	-32.27499090800301	5.72993422503465
C	32.11487092080294	-27.43620135378782	7.22934566927371
C	33.42376511524111	-27.91044336730660	6.64568003145687
C	33.65374991671980	-29.31460262853635	6.90579379765397
O	33.25500943168794	-29.95839577259878	7.87983434719231
O	34.44591279999033	-29.94110880412417	5.95907658408613
H	29.74667650440757	-22.60172957386308	4.50299228339001
H	31.14164231110537	-21.85563652364315	5.29157788381689
H	30.05877815740910	-22.89684964049841	6.21704655617148
H	30.74879745021020	-24.59684658653851	1.70254814590232
H	29.70399531341882	-25.70467206580049	2.59319493421450
H	29.53192743841044	-23.96008677430884	2.81515715317474
H	33.08713847321074	-27.78298386534922	0.13928471078034
H	33.84285556355579	-29.37108195019932	-0.03744708972757
H	32.35188280609312	-29.19679251223845	0.89665916733845
H	35.76995256192041	-30.19916010078523	0.50669803596302

H	37.21046608979230	-29.58949660168766	1.33088524764778
H	36.30095345101429	-30.93302941864744	2.02431956640703
H	34.07308357462682	-22.37549462380493	10.57108842404038
H	32.55338563549606	-22.77299237631964	9.75893704248273
H	33.73403784589106	-21.73419510910084	8.95800855650019
H	37.08929712107555	-24.34055498673473	10.64562784698987
H	35.90169967947048	-25.39342579196494	11.41575895669391
H	39.85786430904771	-29.12509027861068	8.59266169844097
H	39.47644426529648	-27.47160381192697	9.08932270650438
H	38.48986959372305	-28.81534396335151	9.66846526239367
H	38.86197086867856	-30.77041328607622	5.54916629249929
H	39.80081384617061	-29.39219152413846	4.97027929698443
H	40.05224273044584	-30.00657957492979	6.60915706560990
H	35.64311966532715	-23.64472859063869	11.38934330053485
H	33.53743687298339	-32.10082542308956	4.67227460801811
H	34.10247076981913	-33.31008387361378	5.84512419920886
H	32.83644219245376	-32.15051135980956	6.30248292189999
H	34.98491297045691	-31.42393301268717	7.29413973250140
H	35.75785491941278	-31.43562329583660	5.68918437539327
H	32.21756623413663	-26.49242797968003	7.77355441087441
H	31.38962163330372	-27.23863782303482	6.42623151605775
H	31.67752935223038	-28.17746764943130	7.90644367283619
H	31.95541123728325	-26.84549618738592	2.12336392948013
H	37.13626062932452	-26.60628075457790	9.49554197689473
H	37.50885803133276	-29.47428154409434	3.82089569757804
H	32.38161183430686	-23.03067968470858	7.21746685497019
O	35.76837210968939	-25.27932984727059	4.95264189523637
H	35.48820792482062	-25.15822342981677	4.03278469592999

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B3LYP Scan/Hydroxide IPC Model/Triplet/340 degrees Constrained Optimization

C	30.23460099591824	-24.83919341375860	2.71942691616023
C	36.04707712751205	-24.42801789100164	10.78897987799708
C	39.30870817532971	-29.78961006795313	5.89230921273761
C	33.30843581674603	-28.78789108376396	0.72668236352248
N	33.06748358507010	-25.56413084710702	5.07118465114598
N	34.72297029119577	-25.47073718967470	7.43747099355796
C	34.69722229938900	-27.62190858608731	4.01377900875278
C	32.61218871525028	-26.81698751920828	3.02253556946759
C	32.93741297573478	-23.89708252008799	6.86303895852631
C	36.56613545963260	-26.56599778450279	8.60434352940563
C	36.82385018116226	-28.79410288400345	4.32891366261465
C	30.53202437818488	-22.80513668759673	5.24333936977107
C	33.66848653868944	-22.56725302957205	9.57010400256276
C	39.04912487006523	-28.40768503605076	8.82856531806221
C	36.21349279677096	-30.00042046658379	1.53798472813907
C	32.32601127817734	-25.82083150189617	3.95421637134698
C	33.95350677993054	-24.37304949642488	7.68837822844601
C	36.95467941389012	-27.43471538535831	7.58921666725658
C	35.68442244960268	-28.46711149923880	3.59909155366187
C	31.24416487742115	-24.85510914293909	3.82952090788457
C	34.30776460872916	-23.78888959568611	8.97781873853330
C	38.14678536139964	-28.27253565842813	7.63743663157751
C	35.35205004934508	-29.03542318488557	2.29924204195280
C	31.37098522304059	-23.99840391439036	4.89169434978579
C	35.30399274737334	-24.57236644008061	9.49366912101359
C	38.25341128134806	-28.85380502762783	6.40359787225380
C	34.12755755200618	-28.52667666214971	1.95638790769394
C	32.51329860998119	-24.46568473384940	5.66373777496296
C	35.55777435256746	-25.61179240377740	8.50337611583357
C	37.10663039132986	-28.38965963959328	5.63033994805843
C	33.74405652477500	-27.62773904887591	3.03602601723359
N	36.34118661905886	-27.54645758304807	6.37749768482413
Fe	34.67845341070499	-26.59064634922918	5.75075312734001
C	34.73122171772725	-31.31149604241515	6.13311533122832
C	33.71126097252151	-32.15973470706605	5.37951409475756
C	32.15411121964668	-27.41155723432926	7.31343412817044
C	33.42728484824352	-27.91251931416124	6.67621555687397

C	33.58300710892575	-29.34081963958291	6.85120108187692
O	33.02726080188753	-30.05093824197651	7.69510267113287
O	34.48355210622616	-29.91983133804334	5.97316201876948
H	29.72564593699992	-22.65150509444356	4.51787683273622
H	31.12768647101697	-21.88203698469980	5.27067783577926
H	30.06543999108550	-22.91166981649604	6.23236888221286
H	30.70576627092287	-24.68573579354144	1.73812348214615
H	29.68022439658715	-25.78608940244523	2.65987778071723
H	29.49839323482173	-24.03936550750956	2.85553911106468
H	33.07847605385511	-27.86028115156101	0.18415734676999
H	33.83214929359592	-29.45189705018451	0.03019243335324
H	32.34637512719442	-29.26061991465865	0.96909009155936
H	35.77969118181817	-30.24190879824005	0.56111679388178
H	37.21923257142558	-29.59574912854660	1.35887665957398
H	36.34410199215741	-30.94715028474388	2.08038776539898
H	34.11579606961396	-22.30976724787059	10.53661798299402
H	32.59101076696943	-22.70872137654801	9.73484078605493
H	33.77754035142914	-21.69237858834518	8.91409343222919
H	37.12357575779797	-24.27845539194202	10.62567968875230
H	35.94374719840278	-25.32108910276538	11.42114286641354
H	39.87434079307047	-29.10107774409844	8.63230400685022
H	39.49258454400806	-27.44443186207913	9.11802778703753
H	38.50719473748919	-28.78460153069729	9.70709326391494
H	38.88520885872005	-30.75768902742919	5.59045179868457
H	39.82336119661604	-29.37870849970110	5.01242542347198
H	40.07156255058353	-29.99077000462681	6.65266523662163
H	35.68196440838059	-23.57352205055424	11.36954076134867
H	33.66902055076014	-31.86053261428675	4.32803642537070
H	33.97581995037977	-33.22355413732914	5.42689786831977
H	32.72033615922138	-32.02966102496051	5.81844001754785
H	34.72666075148771	-31.56885533209901	7.19527118626698
H	35.73699931814527	-31.46726937422119	5.73092526321309
H	32.30591909451277	-26.48233021297050	7.86951300020853
H	31.40769184765460	-27.17646588482237	6.54022080226860
H	31.71511366165548	-28.15476717038622	7.98602033524257
H	31.93697250537583	-26.91760692854710	2.17780500947910
H	37.15340573088974	-26.57398758856116	9.51788490605031
H	37.53160104956906	-29.47144991537591	3.85934519341603
H	32.39813266266862	-23.01888282060605	7.20608411246590
O	35.77087867839329	-25.29329013605899	4.96747087508223
H	35.47164292521199	-25.16376025704142	4.05481219260847

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B3LYP Scan/Hydroxide IPC Model/Triplet/350 degrees Constrained Optimization

C	30.23741519682414	-24.83393741686286	2.72094135851415
C	36.05204076562529	-24.43255799652449	10.79040186018102
C	39.31869093947535	-29.77468227483171	5.87941676353006
C	33.29264985802393	-28.79914630868636	0.73565132772912
N	33.06315443206120	-25.57244333669824	5.07741431414143
N	34.71967994084546	-25.48137497840095	7.44418739771354
N	34.67940966616707	-27.64460396423588	4.02773375175885
C	32.59980948624897	-26.82903211829423	3.03291263904223
C	32.94231624158011	-23.89976999128089	6.86473846785418
C	36.56665311186016	-26.57345177193805	8.60802404275046
C	36.81202202805277	-28.80753863625041	4.33557364616608
C	30.54730429819131	-22.79485553356133	5.23922667489020
C	33.67752992666424	-22.56801206549152	9.56935468906513
C	39.06663300696984	-28.39426435270255	8.81700132653080
C	36.19751991610102	-30.01457243919324	1.54455850207779
C	32.32031434467878	-25.82766480058033	3.96092254296719
C	33.95494879342780	-24.37959461796047	7.69212773522043
C	36.95515840008807	-27.44005433857264	7.59097553828249
C	35.66707470551200	-28.48838420477568	3.61086239424160
C	31.24563579468862	-24.85431308842351	3.83218864792203
C	34.31224554642488	-23.79328289230980	8.97968083282413
C	38.15400679921353	-28.26916551772177	7.63265558771447
C	35.33403440751927	-29.05472471378161	2.31031848188548
C	31.37785360216632	-23.99522342172571	4.89170061512370

C	35.30656164505065	-24.57850601557885	9.49666616603275
C	38.25752749422094	-28.84972771341981	6.39846773527992
C	34.10982860777720	-28.54405673344761	1.96800070445483
C	32.51615437190862	-24.46837143718268	5.66615443176147
C	35.55648464896051	-25.62102537561736	8.50878796002385
C	37.10202891108336	-28.39485963992960	5.63245493804807
C	33.72704233749530	-27.64641896040793	3.04876806374937
N	36.33601692138873	-27.55568989400958	6.38322613626734
Fe	34.66848834413604	-26.60664133001512	5.76137250951588
C	34.72657411786262	-31.32491259306896	6.22761821444960
C	33.80206545939229	-32.10595571611292	5.29833160342668
C	32.13848474948639	-27.39828114325480	7.31716655584600
C	33.40604174670015	-27.91836517463815	6.68396355418201
C	33.51552110060862	-29.35511537084321	6.83234045970879
O	32.80830906517007	-30.08815330037210	7.53270615830778
O	34.54598528919070	-29.91982835007888	6.10099011223636
H	29.74534794945962	-22.63479937800275	4.51027438837926
H	31.15052342188771	-21.87677280518244	5.26875328095028
H	30.07557486778500	-22.89707599022189	6.22629197942870
H	30.71042060483881	-24.68349541976631	1.74003348611158
H	29.67822833247595	-25.77796433967997	2.66145205894690
H	29.50520639000227	-24.03022985838632	2.85578389255162
H	33.06851185573336	-27.86922013989793	0.19462334826943
H	33.81521076779926	-29.46388785721926	0.03902370043270
H	32.32781864776399	-29.26791966146464	0.97444247914759
H	35.76095338087401	-30.25711717926706	0.56919144819360
H	37.20012746590204	-29.60380382807416	1.36161452296095
H	36.33588721765067	-30.96119967100299	2.08513113792445
H	34.12631070402504	-22.30974126095652	10.53497510495042
H	32.59968086029018	-22.70539911943165	9.73502893965818
H	33.78919612008121	-21.69509814412191	8.91118244584080
H	37.12864633349233	-24.28619558761664	10.62490687589962
H	35.94755762891276	-25.32361311081052	11.42524235205819
H	39.89151372748076	-29.08743394516887	8.61843858287680
H	39.51077997766406	-27.42816710530390	9.09586889572162
H	38.53331481668111	-28.76599026826255	9.70296075303897
H	38.90171504972575	-30.74334850239016	5.57062011209692
H	39.82975423560568	-29.35380892610725	5.00207094835586
H	40.08367213335963	-29.97612878969403	6.63753733156970
H	35.69010928414588	-23.57552999820513	11.36920823600123
H	33.91123808438471	-31.75404119511829	4.26837199483283
H	34.03405823330638	-33.17806398825844	5.32686292584550
H	32.76361205425698	-31.96816450743162	5.60419654508352
H	34.56454077832687	-31.62755680288994	7.26562694534400
H	35.77498818428730	-31.49617804956812	5.96571930934592
H	32.30147851496724	-26.46358707057538	7.85930124106219
H	31.39106266257028	-27.16761159166501	6.54328684608376
H	31.69077789690071	-28.12976333557912	7.99616105480263
H	31.92490193202426	-26.92705814693424	2.18762943777257
H	37.15764937972884	-26.57857685934938	9.51919480492354
H	37.52044108858172	-29.48265168293833	3.86380777545054
H	32.40801008517536	-23.01752254747433	7.20512511868164
O	35.76562724912624	-25.31518123328923	4.97257506478944
H	35.45324521688280	-25.17312611691144	4.06619953519905

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B3LYP Scan/Hydroxide IPC Model/BSS/O degrees Constrained Optimization

C	30.62979191224904	-24.77721374619520	2.31345917057072
C	35.59109721958490	-24.47214435125408	10.92525685131557
C	39.27499581733337	-29.84771048895511	6.36753587905654
C	33.81160099447504	-28.72091672433335	0.63065839177068
N	33.16084540682616	-25.53695830195309	4.97944845689912
N	34.57097760906062	-25.45590819348949	7.45069572423858
N	34.86959705346695	-27.67659105078934	4.07652045762173
C	32.92998139651748	-26.78017356636002	2.88314009520145
C	32.85408590852725	-23.86438300342538	6.73945269575372
C	36.30398482400393	-26.57655247241098	8.76834906337484
C	36.93868360415609	-28.87543806072440	4.57213554498668

C	30.64120929023276	-22.75699386102247	4.86414174668403
C	33.33403733115237	-22.58580323176681	9.53137744985368
C	38.77146753533106	-28.39575597178592	9.23549432073621
C	36.59446506401866	-30.02116334452618	1.70816619541702
C	32.55550442063581	-25.78308151245026	3.78085846553191
C	33.78236080609640	-24.35936215281170	7.65459311900366
C	36.78286281312806	-27.45819958956408	7.80205367175636
C	35.87687225014417	-28.52889790247603	3.74253510579575
C	31.50361922397761	-24.80585469015140	3.53318203416567
C	34.02349417731673	-23.79766255325456	8.97657571692820
C	37.96797255645738	-28.29277922389621	7.97243514803432
C	35.67059857711931	-29.06243265111508	2.40081548079451
C	31.50995703909660	-23.95237712664660	4.60431997686009
C	34.96978039154696	-24.59416964927579	9.56494295482290
C	38.17920284710102	-28.90438187519289	6.76751182677158
C	34.50230540019751	-28.51327454062865	1.94613585496153
C	32.55027069612093	-24.43297642191546	5.50313503501999
C	35.30953694919580	-25.61854187596249	8.58677233169515
C	37.10362855762366	-28.45831467343542	5.88887314483741
C	34.03167585125062	-27.62476747020298	3.00430058244519
N	36.27691059860182	-27.59920193130319	6.54573471985971
Fe	34.68220192474097	-26.61630924773717	5.78563622276782
C	34.50785237038146	-31.37109925603787	6.00351882282449
C	33.69209705661140	-31.98586525620797	4.87109889743994
C	32.11325759896393	-27.4044338572602	7.26744114664905
C	33.35735762445416	-27.90160877270780	6.57189720684895
C	33.36181851183604	-29.36853057578488	6.60066362724046
O	32.49589993676297	-30.08093803301818	7.10735930575403
O	34.44876535471222	-29.94695195801420	5.99402427341143
H	29.92311000294311	-22.59525501152176	4.05242762300232
H	31.23198515663148	-21.83579640924494	4.96684269197702
H	30.06413286525514	-22.86780724808223	5.79293769429339
H	31.21777516611798	-24.65748380891722	1.39274742585251
H	30.05320289518625	-25.70634670036933	2.20301115849004
H	29.91195799040308	-23.95037791063437	2.35204615493681
H	33.69671407325514	-27.77897321611781	0.07617963838129
H	34.36948473407423	-29.41110959319477	-0.01193879878504
H	32.80306901372417	-29.13773682868231	0.76086066152616
H	36.24495342530048	-30.25619122977634	0.69668676891231
H	37.61006006155390	-29.61132674040747	1.61686356831018
H	36.68334131252294	-30.97159513700478	2.25272327035933
H	33.69371465644030	-22.34476476932494	10.53788060490043
H	32.24627004791503	-22.72891597333448	9.59831121533140
H	33.49898232773587	-21.69924046598527	8.90292384007699
H	36.67739104591847	-24.31645844642045	10.86459756990975
H	35.43422309088665	-25.37761990559534	11.52785686369367
H	39.61304550336909	-29.08763672831239	9.11980414318849
H	39.18538670509808	-27.42361560196309	9.53863214283062
H	38.16369709649079	-28.75822834579671	10.07662764212666
H	38.88072396336167	-30.82091712571782	6.04298324512404
H	39.86651756313059	-29.45002812816983	5.53082980330714
H	39.96732995126288	-30.03731553267138	7.19558527854648
H	35.17063884706201	-23.63023668722222	11.48619497839253
H	33.99932713255343	-31.56734161787552	3.90870742869619
H	33.83360061163975	-33.07334680362818	4.84031886522826
H	32.63067227321053	-31.77946524099466	5.01734859314251
H	34.16199343055629	-31.74740093021551	6.97003745376697
H	35.57006587455093	-31.60376835130824	5.88806461527600
H	32.04307323641063	-26.32099291623771	7.28633344059150
H	31.20764590265795	-27.80024036720117	6.78488997023271
H	32.06651141528845	-27.77222259913665	8.30284049501862
H	32.35419088728527	-26.85375511102918	1.96501697540476
H	36.80930886223859	-26.58148527984926	9.72998401982792
H	37.68247058667295	-29.55790466137796	4.17058563047810
H	32.29229134211660	-22.98168405326786	7.03079791302015
O	35.90239605580425	-25.38048031838107	5.06490278605023
H	35.56313639636521	-24.48924162052088	5.23524481088090

B3LYP Scan/Hydroxide IPC Model/BSS/10 degrees Constrained Optimization

C	30.60987716616344	-24.81056046038960	2.32865775826426
C	35.62281567979588	-24.42794992486477	10.90929590629783
C	39.25223171103210	-29.87789275969744	6.39794296609079
C	33.81560572611749	-28.73022262847245	0.64128361860148
N	33.14752475500944	-25.55357355753021	4.99282437298516
N	34.57435804676221	-25.44951160358538	7.45397505251541
N	34.86245678156600	-27.69182297743579	4.09244561037198
C	32.92047588697638	-26.80103065105472	2.89846331979626
C	32.85006731301367	-23.86680489726569	6.74054692322360
C	36.30889787016257	-26.56433760980406	8.77455996610111
C	36.93155938151752	-28.88959197814543	4.59165104912799
C	30.62244411727892	-22.77924555034473	4.87015891437933
C	33.36025885444744	-22.55165070167873	9.50969483326675
C	38.75782781188793	-28.40572297643255	9.25690828311813
C	36.59989033047158	-30.02512319466676	1.72185067240228
C	32.54113879166473	-25.80577630706906	3.79616506892366
C	33.78863885645510	-24.34942461845082	7.65173881984834
C	36.77963768398443	-27.45806070345707	7.81532532496119
C	35.87247783464303	-28.54142167103128	3.75921288966234
C	31.48570559406544	-24.83267157653278	3.54711079750683
C	34.04163673802043	-23.77272184113862	8.96499459042227
C	37.95776632135558	-28.30122185821644	7.99181410533722
C	35.67112483389581	-29.07155442809454	2.41516827744855
C	31.49231009356489	-23.97475648717769	4.61467916749939
C	34.99019072121994	-24.56497099377198	9.55559403943432
C	38.16583131598091	-28.92066806802570	6.79031986111995
C	34.50246034774468	-28.52416482329099	1.95902719204193
C	32.53655385465675	-24.44839030716712	5.51270822293908
C	35.31966712307865	-25.60189591585890	8.58706295159400
C	37.09559865874087	-28.47013929096969	5.90772734960752
C	34.02670228101515	-27.63982241471627	3.01842180507104
N	36.27384879222857	-27.60279999461110	6.55943676702812
Fe	34.67642071605049	-26.62365523680185	5.79707391534924
C	34.47447963827270	-31.37741114767980	5.96978543692115
C	33.75278522606731	-31.88882564281734	4.72755450330138
C	32.14713745625086	-27.41291146819620	7.35013562217139
C	33.35625635154420	-27.90825208791280	6.59401797385072
C	33.31842480710597	-29.37350082093295	6.53951061954003
O	32.36987806446734	-30.08317803965050	6.87224993993799
O	34.46384568238548	-29.95410673039906	6.05667184862890
H	29.90322570239675	-22.62220469238923	4.05852067058823
H	31.21239119850418	-21.85694122992269	4.96755206943348
H	30.04667431060247	-22.88618741020223	5.80021512259417
H	31.19644004316608	-24.69467059411197	1.40655642113057
H	30.03383787041079	-25.74061354825993	2.22349947796124
H	29.89156931869100	-23.98401095798784	2.36443585873212
H	33.70070936572103	-27.78729688144274	0.08853204175217
H	34.37621571615227	-29.41828209374527	-0.00121166650026
H	32.80752944678694	-29.14907256656161	0.76820916195991
H	36.25290256123175	-30.25911858220475	0.70928969676226
H	37.61396759104927	-29.61100042914113	1.63361758083232
H	36.69132446162568	-30.97657162379639	2.26419396496158
H	33.72862355810550	-22.29864721464356	10.51010384244437
H	32.27260610615306	-22.69038201338079	9.58701096831142
H	33.52292309421004	-21.67390382486107	8.86840613711630
H	36.70938792088809	-24.27906754834996	10.83803081407269
H	35.46589854736180	-25.32414061494219	11.52567908908962
H	39.59363071883242	-29.10530553925360	9.14573565481062
H	39.17963373867095	-27.43598529242909	9.55696249099540
H	38.14534088883975	-28.75954180508461	10.09831195912748
H	38.84763553583601	-30.84863597621934	6.07878804867180
H	39.84964837210486	-29.49228376935651	5.55975886907335
H	39.94103392524502	-30.06989710022287	7.22837776497258
H	35.21117912352046	-23.57619291947421	11.46184840582588
H	34.15854062012360	-31.41905636249250	3.82790564149839
H	33.86853245701973	-32.97613058188973	4.63754641967974

H	32.68861537780452	-31.65805886939345	4.79047482056521
H	34.02743775379381	-31.80467154810814	6.87198040495991
H	35.53534380461441	-31.64031815554282	5.93793679823250
H	32.09159000114101	-26.32925084307324	7.39501191477574
H	31.21949114440331	-27.79028846285464	6.89782561894670
H	32.14000347213788	-27.79898532435162	8.38090305542887
H	32.34495120878507	-26.87707671532094	1.98039215486797
H	36.81701191820314	-26.56337092814952	9.73477537810925
H	37.67401627747497	-29.57497135386481	4.19264149538302
H	32.28930145889870	-22.98198382876861	7.02745522334610
O	35.89252256310643	-25.39028390271694	5.06490643993232
H	35.57851961372497	-24.49828153015033	5.27498875086605

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B3LYP Scan/Hydroxide IPC Model/BSS/20 degrees Constrained Optimization

C	30.59042572882504	-24.83136752114871	2.34627418226312
C	35.65210991433813	-24.40428906454645	10.89678323463832
C	39.23531684802737	-29.90104718960835	6.40776169167311
C	33.81665149108894	-28.72404703908460	0.64161144892985
N	33.14171782111089	-25.56034737993231	5.00103448616447
N	34.58072532952418	-25.44590012256472	7.45437242373614
N	34.85180794632507	-27.70443915904234	4.10216752201078
C	32.91226081799496	-26.80929635862202	2.90742198229258
C	32.85071953790577	-23.86780852165980	6.74389609637126
C	36.31756733998932	-26.55833647055259	8.77447787219602
C	36.91802704107632	-28.90674659581644	4.60213333859188
C	30.60675898551593	-22.79504993346156	4.88376601289624
C	33.38223545382106	-22.53413857625359	9.50003871270927
C	38.75877951229146	-28.40965946371969	9.25965839013022
C	36.59947972366110	-30.02016390885306	1.72045345114896
C	32.53184078074805	-25.81618822991686	3.80689699773746
C	33.79687353651101	-24.34397870105682	7.65064998636382
C	36.77897804864374	-27.46174899606952	7.81992224789595
C	35.86232768775736	-28.55349278471666	3.76756482258088
C	31.47192839375488	-24.84732482299534	3.56069526337526
C	34.05879018495615	-23.75939274587017	8.95874300091153
C	37.95361660201608	-28.30968034540935	7.99742676596800
C	35.66630785124686	-29.07461642773454	2.41910908687332
C	31.47993605858820	-23.98773295037887	4.62682638091356
C	35.01014729095857	-24.54906380900117	9.54827484671061
C	38.15429079218472	-28.93730115326126	6.79902811084992
C	34.49900728320274	-28.52486023896506	1.96260410807049
C	32.52995188446820	-24.45592011195864	5.52105655395668
C	35.33182930132881	-25.59283748494752	8.58450452507770
C	37.08370141315964	-28.48586899227426	5.91738604606652
C	34.01928026265134	-27.64720422788339	3.02542348481247
N	36.26780067416346	-27.61154140466654	6.56688639984095
Fe	34.67146947826712	-26.62919518271674	5.80440210109019
C	34.40772393688626	-31.39640754822173	6.02233896570178
C	33.87653924828044	-31.84299984880379	4.66474649622114
C	32.15091639197217	-27.40747689342609	7.37988880259590
C	33.34531735833114	-27.90251091331091	6.59889694837092
C	33.25493218961360	-29.35913017788528	6.45903505842700
O	32.23230437378071	-30.03114582256868	6.58148479369037
O	34.44317500287008	-29.97569501396293	6.15761560119169
H	29.88167093472907	-22.64409855628103	4.07619614307277
H	31.19330459934793	-21.86982952133118	4.97393442495470
H	30.03741044024397	-22.90112345388985	5.81784864680252
H	31.17193286386445	-24.71231920926098	1.42133620659686
H	30.02003641756801	-25.76521312779366	2.24450632487304
H	29.86706957391644	-24.00937101563623	2.38486643902517
H	33.69562515769304	-27.77706477507070	0.09732014776136
H	34.38387888649387	-29.40197153612138	-0.00584763641536
H	32.81169662584639	-29.15208215006065	0.76271511075581
H	36.26376323561359	-30.23439607187334	0.69977160102507
H	37.61592796018584	-29.60833052206851	1.65195534825807
H	36.68124561426057	-30.98227225826741	2.24551283494892
H	33.75478393155958	-22.27728594453111	10.49792008447604

H	32.29455951894818	-22.67001738103341	9.58190138410122
H	33.54449780322246	-21.65976004272435	8.85404550209725
H	36.73808411487734	-24.25515169254817	10.81714987925335
H	35.50022189268982	-25.29725232111575	11.51910070525405
H	39.59045422961629	-29.11434328547050	9.14950549321300
H	39.18723827235665	-27.44014767265482	9.55099611707129
H	38.14851911187638	-28.75434135043262	10.10645433602928
H	38.82502484049997	-30.86946644395566	6.08899160363958
H	39.83545834339487	-29.51965030475457	5.56952559913375
H	39.92277402316970	-30.09651868326034	7.23852853977642
H	35.24380929919210	-23.54983114583648	11.44764168994072
H	34.43993580141326	-31.37008639913809	3.85708303676199
H	33.96100838558068	-32.93203762436797	4.56073148709903
H	32.82733515980096	-31.56362712707739	4.56357739737351
H	33.80144243720920	-31.82562897005977	6.82546570205945
H	35.44736577694608	-31.70830753188848	6.15469447099727
H	32.13463337838483	-26.32715745191474	7.48956097650596
H	31.21497813445232	-27.7238883372605	6.89974610432743
H	32.12314309193233	-27.85216172968663	8.38707538898590
H	32.33636347743323	-26.88465939419510	1.98957479907549
H	36.83031369780290	-26.55259420751570	9.73221842338822
H	37.65821581567796	-29.59503697028578	4.20396446408413
H	32.29056325088224	-22.98240621235645	7.03016438139111
O	35.89075206641880	-25.40419581677147	5.06471101871084
H	35.59840832106152	-24.51044821217525	5.29723248054849

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B3LYP Scan/Hydroxide IPC Model/BSS/30 degrees Constrained Optimization

C	30.59054562398799	-24.85949324083282	2.33937824369413
C	35.67805483416500	-24.36250076315076	10.87423445230997
C	39.22150924474291	-29.92745742406532	6.43954497871386
C	33.87270180604081	-28.69627373868427	0.62115533318166
N	33.13702191070347	-25.57855060534434	5.00141560254578
N	34.57741649630156	-25.44890059616886	7.45399223963070
N	34.85630704823128	-27.71856601084580	4.10924541789296
C	32.93166021103359	-26.81414463867850	2.89765717525863
C	32.82630726646124	-23.89309632769460	6.74851531380754
C	36.32729054060960	-26.54252594155020	8.77475073415546
C	36.91191848027299	-28.93321658269659	4.62539869759985
C	30.56853000282776	-22.84379243971516	4.89306262787239
C	33.36994313385606	-22.53153332985259	9.48675228628453
C	38.76592392019160	-28.39484845208453	9.27268609351521
C	36.63655659920539	-30.00989830419094	1.72718708097016
C	32.53653490061360	-25.83190244692753	3.80213594836742
C	33.78404100750416	-24.35391414600270	7.65002987732162
C	36.78047523505274	-27.46116406953100	7.83091265938406
C	35.86888844107300	-28.56797232899612	3.78060004034034
C	31.46702949133158	-24.87342313379257	3.55739652903089
C	34.05287668979093	-23.75539040264553	8.95007353983953
C	37.95297483962197	-28.31062566798447	8.01422236681745
C	35.69201525141076	-29.07410025459686	2.42370620700401
C	31.45878957223091	-24.02250009965419	4.63026825659053
C	35.01939885518300	-24.52917513172417	9.53619539920917
C	38.14514394862685	-28.95571479142242	6.82364892881607
C	34.53345684177607	-28.51627148933179	1.95570337774206
C	32.51090312833655	-24.48414595906440	5.52576941066845
C	35.33994124764338	-25.57958138209677	8.57904375589871
C	37.07356881111883	-28.51049163465325	5.94046081305015
C	34.03949845116004	-27.64965901112894	3.02115423868886
N	36.26258029457221	-27.62617506872311	6.58243801567960
Fe	34.6677297214131	-26.64217624597459	5.80923921048141
C	34.27273033935674	-31.42077335202023	5.94393302983949
C	33.80679966491840	-31.78909707947674	4.54018789836535
C	32.26522461272143	-27.40046058317128	7.55043972769426
C	33.34701243525844	-27.90953636897958	6.62726094852925
C	33.19241830967282	-29.34858758655542	6.40333323013925
O	32.13194835077225	-29.97118858216709	6.41340498445287
O	34.36690949709182	-30.00949493425396	6.14402089694511

H 29.85474963966085	-22.68712015656968	4.07659011174645
H 31.14339850422667	-21.91410301429142	5.00818150055321
H 29.98561239025872	-22.97172023918665	5.81606526567769
H 31.17630823249944	-24.74381689382476	1.41680612630893
H 30.01910637386732	-25.79274031146574	2.23783521042469
H 29.86839740902398	-24.03620508318338	2.37286566565385
H 33.78421503705349	-27.74534853192421	0.07726924976047
H 34.43672752023333	-29.38549941826701	-0.01705277946608
H 32.85610612341887	-29.10134628215954	0.72170189232792
H 36.30474033525431	-30.22860044907379	0.70620518153133
H 37.64842622216324	-29.58653132575575	1.65981000635179
H 36.72840566183157	-30.97047702693147	2.25315197075805
H 33.76164375652465	-22.25161927123677	10.47103919114922
H 32.28664800491782	-22.68239654070269	9.59659220575201
H 33.50343722763439	-21.66622782443188	8.82240848895237
H 36.76156991549041	-24.20551132553256	10.77782763254573
H 35.54232765365020	-25.24844300990011	11.51020521901533
H 39.59420937523264	-29.10425364984010	9.16738546807803
H 39.20010467701140	-27.42274540583884	9.54646953369981
H 38.16028177565158	-28.72442060432919	10.12872351715592
H 38.80654201987078	-30.89751069062721	6.13209784704846
H 39.82057720819460	-29.55708504943466	5.59557214525476
H 39.91085725235114	-30.11650841543940	7.27023593369667
H 35.27013400743523	-23.50441216656028	11.41968579017590
H 34.44074103328561	-31.31597920099953	3.78723562741290
H 33.84595632802721	-32.87656786112450	4.39917393625308
H 32.78059776350315	-31.45399390890037	4.38729425942942
H 33.59905383072064	-31.85080659312121	6.69099973646558
H 35.28663230093548	-31.78797524635737	6.12589143365793
H 31.90485307385510	-26.41173332993422	7.26246756287972
H 31.41417728288098	-28.08664193957087	7.60569212192734
H 32.66918549670015	-27.29086565615909	8.56874812012470
H 32.36533803083287	-26.88464198108155	1.97353689077989
H 36.84654738106995	-26.52388710932389	9.72882295073834
H 37.65166526477887	-29.62464287883637	4.23188688326201
H 32.25618999141803	-23.01434637457037	7.03564586269859
O 35.89088133321685	-25.42210220696190	5.06714912480795
H 35.64009347170699	-24.53287946012147	5.35816244508132

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B3LYP Scan/Hydroxide IPC Model/BSS/40 degrees Constrained Optimization		
C 30.58768514972650	-24.78670166316425	2.32710948585281
C 35.65114385975463	-24.42015685915599	10.88012530987196
C 39.16846538772475	-29.96662014279855	6.38960682958676
C 33.81851734788449	-28.65872949467050	0.59087481005501
N 33.13492256988820	-25.53848820399769	4.97945058290406
N 34.57383475968936	-25.44091375795764	7.43270833332109
N 34.83404339102653	-27.69102165259082	4.07241083854093
C 32.91354430380092	-26.76328451659081	2.87083694996442
C 32.83350611784643	-23.86683873795360	6.74112779399670
C 36.31131868605275	-26.56309948908832	8.74577655600156
C 36.88045765193982	-28.92514317989125	4.57679827353499
C 30.58320268985601	-22.78707873151969	4.89355555665674
C 33.36456481738551	-22.55331179238156	9.50640132313468
C 38.72117489561987	-28.45507076763432	9.23631607980417
C 36.57049253319911	-30.00684556687924	1.68203858265367
C 32.52950491469417	-25.78147833218320	3.780751651135014
C 33.78469264650305	-24.34514439142500	7.64097684424645
C 36.76290599332057	-27.47128260625038	7.79112587011969
C 35.83563686419941	-28.55144004637379	3.73721438510714
C 31.46630396901023	-24.81371704242859	3.54326059507611
C 34.04734046845901	-23.76943868472617	8.95255871852369
C 37.92085752393641	-28.34099105361108	7.97237492965954
C 35.64470856979566	-29.05521972452653	2.38168449789529
C 31.46555142371582	-23.96953554784573	4.62141372412910
C 35.00559547564889	-24.55791046327377	9.53259567277067
C 38.10992734430150	-28.97670048935954	6.77640302047352
C 34.49100182659421	-28.48286094807757	1.91994915945092

C	32.51593992208529	-24.44412346436551	5.51223304055496
C	35.32858228162689	-25.59340746884146	8.56021949562482
C	37.05079348252438	-28.50503603908610	5.89174907046821
C	34.01232433115027	-27.61141837005964	2.98806403944754
N	36.25194069393044	-27.61287023292159	6.53709805655444
Fe	34.65972921863671	-26.61871586065358	5.77819540655862
C	34.34622424695335	-31.42546641151190	6.22321156669208
C	34.14320716751359	-31.88064180257539	4.78270945835244
C	32.22397769827938	-27.40206534916769	7.47003704957208
C	33.34622948649638	-27.88372113931954	6.58009444920222
C	33.22634211217628	-29.32804292081553	6.35841439857016
O	32.17892970096116	-29.93952688406130	6.16997306138444
O	34.42206117583913	-30.00312400409294	6.35786390671056
H	29.86410648040756	-22.62475889248792	4.08281782224024
H	31.16300672679469	-21.86018176786640	5.00697830504554
H	30.00622432137871	-22.91460090985720	5.82034447633430
H	31.17172002051795	-24.66355628379181	1.40434649718122
H	30.01436586400212	-25.71793819990465	2.21808663125819
H	29.86698911166321	-23.96250709081185	2.36941421222854
H	33.69870277399345	-27.70187809610942	0.06406444316888
H	34.39213362044589	-29.32262100890180	-0.06548074979992
H	32.81382217906850	-29.09177182731491	0.69648381806093
H	36.25238648804868	-30.19004932155990	0.64971012268932
H	37.59720742696810	-29.61723553176974	1.64490796224124
H	36.61995746355137	-30.98328887355832	2.18489231209482
H	33.74502402613658	-22.29728602414952	10.50154520724989
H	32.27909442039417	-22.70014159731884	9.59918413859533
H	33.51123334032447	-21.67450295255066	8.862803529994729
H	36.73714166849368	-24.27261303706239	10.79844374650276
H	35.49956675015103	-25.31552003518047	11.49924054089690
H	39.54442324699652	-29.16961570262351	9.12596387514276
H	39.16106182787010	-27.49202612388119	9.53205670632238
H	38.10471168049214	-28.79499003610240	10.08062227996509
H	38.73485814077726	-30.92555599202449	6.07309134968664
H	39.77897158994308	-29.60290765169726	5.55091774024358
H	39.85008883867191	-30.17623002367387	7.22176437762363
H	35.24558298416878	-23.56754805719958	11.43591781074445
H	34.91948492432788	-31.46640916200550	4.13633516681022
H	34.18280827037146	-32.97555758777780	4.72139688733481
H	33.17350666349709	-31.54541523907251	4.41570879333075
H	33.53984428384749	-31.80805808883138	6.85606525836324
H	35.30240596703275	-31.78501251373302	6.61329889498781
H	31.96886761919223	-26.35692834634950	7.30180250365621
H	31.32303278176566	-28.01375829086387	7.34520387770587
H	32.52147854920013	-27.48300813637368	8.52884348242439
H	32.34257499111388	-26.82592296687360	1.94901940552118
H	36.82397629621094	-26.56320325591252	9.70359840263198
H	37.61018743662113	-29.62574505034726	4.18075263969643
H	32.26770555514505	-22.98816369725067	7.03695270461873
O	35.88689673972241	-25.39859447383887	5.04151273884014
H	35.62468223494463	-24.50774089954378	5.31701761203978

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B3LYP Scan/Hydroxide IPC Model/BSS/50 degrees Constrained Optimization

C	30.62219621660895	-24.65946491204011	2.29782613823596
C	35.63560474825859	-24.49164746707806	10.888483393592596
C	39.13709348855453	-29.98290907625383	6.31249781916795
C	33.74683960711594	-28.61515155110279	0.55841377352549
N	33.12848634932543	-25.49865279810766	4.96335307006987
N	34.55564923350475	-25.45392882565310	7.42530650367799
N	34.79920669774250	-27.66866229452885	4.03448642079441
C	32.90253312817776	-26.68935691256410	2.83553703228779
C	32.82343996774359	-23.86136210577456	6.75686115227892
C	36.30424274446187	-26.58893348128717	8.71108444368946
C	36.82445915379336	-28.94046469084128	4.52888609165543
C	30.61035108183858	-22.71501850544488	4.90706062537056
C	33.34171842926876	-22.60764148661049	9.55256787201022
C	38.72366219626579	-28.47392487327951	9.16573917286392

C	36.45044886652416	-30.05315007166531	1.65163339242210
C	32.53197771737361	-25.71038773312200	3.75413459959111
C	33.76579507688883	-24.36297572770286	7.65317810990909
C	36.75223052533057	-27.48382619458349	7.74303312750701
C	35.77632036189815	-28.55619444930831	3.69748964464037
C	31.48509415335842	-24.72327914857281	3.52378557194358
C	34.02732529817308	-23.81131697719752	8.97545010412866
C	37.91053636968763	-28.35637327952712	7.91027587807063
C	35.56452008809132	-29.06089864701784	2.34560127503969
C	31.48159040628108	-23.90212076045532	4.61936449524984
C	34.98937641016396	-24.6066622235600	9.53915421683822
C	38.08527141421102	-28.99083648670663	6.71178144141817
C	34.42830202054505	-28.45409091472331	1.88478512579315
C	32.51616701687924	-24.40767386328193	5.51156513711443
C	35.31400149937271	-25.62319174336105	8.54741881086534
C	37.01773730169824	-28.51438956342417	5.83922954508023
C	33.97746707828242	-27.56691897789553	2.95169662470955
N	36.23048754485033	-27.61850743976479	6.49276510559825
Fe	34.64047628918016	-26.60858157685350	5.75068663527861
C	34.34589596358163	-31.43781570701465	6.53380583830048
C	34.61344759599319	-31.94511150344148	5.12250827947614
C	32.12474104203035	-27.42363449158680	7.31214985400718
C	33.32640752555830	-27.87848582247730	6.51631121529229
C	33.25247359469010	-29.33097568516824	6.30239225036354
O	32.27857452918206	-29.93669780797446	5.87523220934472
O	34.39964400699314	-30.00973049096923	6.63522942480929
H	29.89730634505127	-22.53088756950822	4.09563166428914
H	31.19934193108065	-21.79644355131624	5.03964331719914
H	30.02714811998847	-22.85257699725806	5.82848329473260
H	31.21958628018425	-24.52340987184232	1.38546330558472
H	30.03963136267647	-25.58130323004390	2.16125045808558
H	29.91070373777072	-23.82781742368832	2.34898810703580
H	33.64979262325171	-27.65622768235279	0.03061943421741
H	34.30160450238437	-29.29410937411513	-0.09863155216305
H	32.73184144969003	-29.02211504441397	0.66853367813352
H	36.13445369770384	-30.21780594831692	0.61547728335878
H	37.49562529931116	-29.71521642859612	1.62512444202500
H	36.44436468363111	-31.03119256843215	2.15351986760543
H	33.72187227568580	-22.36976529039557	10.55231484089507
H	32.25658304329640	-22.75870123608805	9.64250045573310
H	33.48630497729815	-21.71629925712242	8.92589270219319
H	36.72137440344628	-24.34129301427858	10.80863602760401
H	35.48571075948234	-25.39804579715010	11.49173449772735
H	39.54845459193562	-29.18480871279219	9.04401444813898
H	39.16234981288533	-27.51051137956735	9.46185852115583
H	38.11652087205892	-28.82034523659559	10.01417502488132
H	38.69975473262144	-30.94792613798995	6.01996643631753
H	39.72538192049731	-29.62825332890701	5.45444020884785
H	39.83968213704323	-30.17887624154604	7.13049569818870
H	35.22938694909465	-23.64930630547875	11.45931164306872
H	35.57545438893798	-31.57915772511987	4.75785252664006
H	34.62963169017166	-33.04221018858090	5.11176642537602
H	33.83306138896805	-31.60113665334953	4.44280609816149
H	33.37015204901176	-31.78757616410314	6.88206368375444
H	35.11796960571172	-31.78781114562751	7.22472530232570
H	31.94770131609439	-26.35283363885916	7.23725405861756
H	31.21792365339745	-27.95523499482581	6.99564792803596
H	32.26399144455642	-27.65158693936088	8.38286101301033
H	32.33596582908437	-26.72980501684074	1.90970702964591
H	36.82364325941733	-26.59928545396103	9.66526651059991
H	37.54195882310430	-29.65048155641966	4.12715248178710
H	32.26073219274354	-22.98547543224262	7.06655647548648
O	35.87481123929324	-25.38331400480064	5.03084825787785
H	35.57744987595908	-24.48993377139473	5.25822133747978

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B3LYP Scan/Hydroxide IPC Model/BSS/60 degrees Constrained Optimization
C 30.64287667685486 -24.56754247960658 2.27841579833432

C	35.63349202014852	-24.54862417738380	10.88484053716413
C	39.11634493683994	-29.99942485034873	6.24140600621463
C	33.70825056961890	-28.55824831460491	0.51619755919506
N	33.12746075612619	-25.46755786907641	4.94542494801516
N	34.55015811555409	-25.46361983558898	7.40976351442404
N	34.78826454354186	-27.63672203396178	3.98994079405081
C	32.90555289589265	-26.62266340517015	2.79743266301381
C	32.80860667418001	-23.86869546459646	6.77050645749774
C	36.31220296988737	-26.60432516333613	8.67148870210212
C	36.78769893306175	-28.95059870949774	4.47939612591434
C	30.61089142649809	-22.68126798864761	4.92927323220498
C	33.31652771894011	-22.66536073381815	9.58925922862169
C	38.73029660557912	-28.49326120344963	9.09958442980285
C	36.37698700847468	-30.06323776633381	1.60688866732715
C	32.53843742903494	-25.65400093910869	3.72819161372765
C	33.75169952333593	-24.38348325587759	7.65849625290437
C	36.75450457837702	-27.49079049312329	7.69335770727305
C	35.74434478655931	-28.54616075875592	3.65100390232014
C	31.49499968415217	-24.66020467881658	3.50998127823414
C	34.01185323394051	-23.85218609697903	8.98939848342455
C	37.90878451096738	-28.36991624902337	7.85020886196441
C	35.51798090727201	-29.04711402622170	2.30004394751826
C	31.48305812930508	-23.86311710381898	4.62316200918851
C	34.98424728454294	-24.64687049358954	9.53572571613300
C	38.06968775894021	-29.00567079718259	6.65050309085172
C	34.39688686112341	-28.41245699938476	1.84050302318788
C	32.51086160162212	-24.38816027062840	5.51168569415031
C	35.31447129447685	-25.64374145349867	8.52599309679542
C	36.99790698071975	-28.52220961219962	5.78679492519742
C	33.96681874470030	-27.51707484867002	2.90895932088344
N	36.22378343118825	-27.61831021221807	6.44577117789558
Fe	34.63663622845441	-26.59448480508611	5.71977542733180
C	34.30802315308949	-31.42842268735061	6.81552692792610
C	34.88609625128878	-31.98990132207991	5.52327588409761
C	32.06445567524975	-27.46547611159804	7.15837924177007
C	33.33438390356674	-27.87636022061978	6.45067282663809
C	33.32282949664774	-29.33329755577540	6.24164246289079
O	32.48568532896154	-29.95052080458107	5.60235017396922
O	34.34781710224247	-29.99561540830353	6.87511185719369
H	29.89531158838064	-22.48720966584258	4.12235389326365
H	31.19851942657152	-21.76334902705116	5.07271429555471
H	30.03031737931408	-22.83214092935092	5.85024455566187
H	31.24700261117286	-24.39761194773839	1.37612559240023
H	30.07103105620151	-25.49045117196057	2.10814228477570
H	29.92247311680692	-23.74494173022818	2.34827553855319
H	33.63809964803944	-27.59880140840743	-0.01513270084822
H	34.24130325467028	-29.25553787267482	-0.13955219141618
H	32.68207131523042	-28.93471512198617	0.63071651195382
H	36.04141438850291	-30.23861804020358	0.57866751610047
H	37.42709901312279	-29.74296401773196	1.55816379220753
H	36.36359829259587	-31.03268867871099	2.12475495356123
H	33.69113137328168	-22.44659099239066	10.59545445516544
H	32.23199002589882	-22.82490684069700	9.67141367391363
H	33.45791261340501	-21.75968087754158	8.98261861410701
H	36.71690094470106	-24.38222858226348	10.80452663505359
H	35.49779931166543	-25.46831663781525	11.47107145095233
H	39.54986183075785	-29.20911240748139	8.97187171797999
H	39.17674746901189	-27.53272385129277	9.39336792016706
H	38.12676715228968	-28.83654686876798	9.95185253090938
H	38.67726776707423	-30.96438321116166	5.95104166908945
H	39.69811273733625	-29.64404901463755	5.37925106329453
H	39.82509766604917	-30.19716532800787	7.05364386566823
H	35.21791435762074	-23.72278976924612	11.47286539498670
H	35.90526772980319	-31.62985525458325	5.36852509603216
H	34.90308194579792	-33.08623341642705	5.56195088246683
H	34.27838350366706	-31.67931832612232	4.67304360565402
H	33.27524924299266	-31.76446008832860	6.94351434734046
H	34.89769229967177	-31.75147982861300	7.67794456307334

H	31.94583023406477	-26.38602535307214	7.21798606207882
H	31.18430479453102	-27.88418375678270	6.64897076364694
H	32.04004431541087	-27.85919395634115	8.18908832249717
H	32.34151113297324	-26.64668404768372	1.86944013103943
H	36.83703128837910	-26.62303589721115	9.62253354455666
H	37.48904025646199	-29.67568616561793	4.07620729613078
H	32.24128931547799	-23.00173584470487	7.09656016633947
O	35.87066675951439	-25.35974053829052	5.01150183373109
H	35.55001311459527	-24.46817291311919	5.21288168300735

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B3LYP Scan/Hydroxide IPC Model/BSS/70 degrees Constrained Optimization

C	30.65540257263228	-24.62659561259859	2.26906542740337
C	35.59627184399668	-24.51314372145656	10.90568551363982
C	39.11362481399500	-30.01063628847102	6.34349237360476
C	33.85233480425357	-28.51087647069890	0.50201702332029
N	33.12991968873931	-25.48811646965350	4.95706223868221
N	34.54029606033856	-25.46043276431564	7.43028714991018
N	34.83698988358879	-27.62851894594197	4.01463060024722
C	32.96551470370000	-26.62654949523315	2.79547935751597
C	32.76930355183099	-23.90025255620470	6.78238743404842
C	36.29812230158376	-26.58332224035680	8.71518624035399
C	36.82727595452320	-28.94387233440322	4.53829746373764
C	30.54877572090788	-22.76303976310074	4.93375185541237
C	33.26084454829630	-22.66644188352156	9.59023080601938
C	38.70460341691992	-28.47972686599484	9.18458887624319
C	36.50454199731715	-30.01010846220447	1.63930144414024
C	32.56108558862310	-25.67806017280459	3.73123253419589
C	33.72447523966557	-24.39038355452246	7.67134246626616
C	36.74738543060244	-27.48032848966637	7.75000577832183
C	35.80630806891318	-28.52839768917867	3.68805984654778
C	31.49635249144439	-24.70794134934571	3.50918297610277
C	33.97290029115885	-23.84826735763736	9.00013399623606
C	37.89708952798622	-28.36157448404455	7.92556456591768
C	35.61786968121502	-29.01278010963959	2.32514912947962
C	31.45263412744690	-23.92095366638431	4.62865942091833
C	34.95323021456313	-24.62733092543048	9.55480516135956
C	38.06860083551835	-29.00716345942358	6.73239150594837
C	34.50381690720091	-28.38025204402201	1.84645445769021
C	32.48426288277463	-24.42756927121881	5.52388787199224
C	35.29914598077127	-25.62658054969796	8.55299088971816
C	37.01040590483095	-28.52439467155436	5.85244413664419
C	34.03975257004734	-27.50359146725750	2.91652079671818
N	36.22910560784437	-27.61590353992008	6.49753495546156
Fe	34.64689801766034	-26.59450492277126	5.74393048825310
C	34.06722672748963	-31.50807568459579	6.53460487435830
C	34.78603060009110	-31.97910879203331	5.27797767469093
C	32.14223677678524	-27.51881199770659	7.28228148211920
C	33.34463006000453	-27.88104209311643	6.44349748627338
C	33.26638353267631	-29.30531854849078	6.07541021541517
O	32.46704380453460	-29.79479750759443	5.29686675073523
O	34.17695053702209	-30.09209827463071	6.74194613796368
H	29.83841201677487	-22.57977635534654	4.11969484350721
H	31.11230434975107	-21.83238813237082	5.09126091623386
H	29.96118438120025	-22.93517259112980	5.84656304005552
H	31.26502733248405	-24.43484415755301	1.37481815623572
H	30.10851469929963	-25.56197416779527	2.08561283328238
H	29.91445272156586	-23.82228847210452	2.33724821831067
H	33.79090865669156	-27.54417829543566	-0.01702935066157
H	34.40745729778671	-29.19551675179851	-0.14883996922876
H	32.82600753469769	-28.89540958529643	0.58317622965724
H	36.20974888879273	-30.15801520947547	0.59438372019164
H	37.55489892242934	-29.68743208370199	1.64014785064147
H	36.47318130185412	-30.99341422435765	2.12980472060870
H	33.62843492807408	-22.43732502182955	10.59670277735032
H	32.17795291847939	-22.83844099987900	9.66873560422543
H	33.39396929479454	-21.76283459429359	8.97867870609145
H	36.67736538741617	-24.33079982214799	10.82833242410400

H	35.47241674709869	-25.43212563667800	11.49563526868922
H	39.52750773771573	-29.19357063972638	9.06747825118731
H	39.14512091283557	-27.51728241888813	9.48099346323260
H	38.09269944620605	-28.82285907281081	10.03099397705735
H	38.67108828371288	-30.97559679158539	6.05836251880996
H	39.70609773219812	-29.66766931569873	5.48360611697344
H	39.81310379539371	-30.20448081369709	7.16464655424704
H	35.16632851862341	-23.69104557948914	11.48853325352789
H	35.83441104519170	-31.67389262353991	5.29544401524544
H	34.73986895477117	-33.07270825012835	5.20345284244597
H	34.31852585565067	-31.54806608543410	4.39220238215818
H	33.01000387415210	-31.78333803349704	6.49203109729815
H	34.51506864284308	-31.95001635588175	7.42911328001452
H	32.09010560652447	-26.45567410503753	7.50729397734540
H	31.21028269883514	-27.81007936075031	6.77372724307083
H	32.15096263280912	-28.06271593293717	8.24260099430485
H	32.41834101718209	-26.65084366288330	1.85748459328984
H	36.81504560761846	-26.59286644792006	9.67068571342844
H	37.53673733189209	-29.66678497109531	4.14557986277796
H	32.18369439236297	-23.04445143185805	7.10572519521713
O	35.87324231513106	-25.34915800836299	5.03751496266350
H	35.60807692766580	-24.46801982774168	5.34005009516604

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B3LYP Scan/Hydroxide IPC Model/BSS/80 degrees Constrained Optimization

C	30.70980598519453	-24.41576216210129	2.21121849811464
C	35.52646914795130	-24.73793751934470	10.91074991895430
C	39.06397092287712	-30.05328197445067	6.14247886566423
C	33.80576757358694	-28.33867652279781	0.35773620258618
N	33.12659890947589	-25.43394776864721	4.89843848074526
N	34.50480785851423	-25.52270904410062	7.38571203549403
N	34.79739508573537	-27.57745422652943	3.89633359337303
C	32.96309104682943	-26.48959417433880	2.69427362443915
C	32.75262826902415	-23.92345447741390	6.78690029200889
C	36.25788125187034	-26.69810873750441	8.62958630762392
C	36.74991043053891	-28.95757154746632	4.39051176134078
C	30.59134751322212	-22.66476166519602	4.95059767663196
C	33.20011029887100	-22.83600048066299	9.66140230044856
C	38.66859999047595	-28.60284519597469	9.03046916804794
C	36.39025439769161	-29.96385160443992	1.47545773397659
C	32.57124330594326	-25.56378026468299	3.65806044655937
C	33.68720471744020	-24.46569265238949	7.66769110892510
C	36.70727650346929	-27.56062235791654	7.63348095748790
C	35.73737193522584	-28.50093432325685	3.55231203356884
C	31.52810290629742	-24.56535320071115	3.45996360480199
C	33.92148988354685	-23.98642328389286	9.02285835974126
C	37.85272668042099	-28.45234027903403	7.78036198798636
C	35.53877046880757	-28.94816506883343	2.17809115231614
C	31.47991750940629	-23.82486562997218	4.61057049825621
C	34.89907598748283	-24.78809101981460	9.54886904112682
C	38.01550074367609	-29.06842766159656	6.56960928354782
C	34.45211300970462	-28.26500529967893	1.70884322951080
C	32.48817916389738	-24.38603697939092	5.49918128406993
C	35.25629236319399	-25.73890875205277	8.50457303127477
C	36.95358600585620	-28.55896857271784	5.70888585977980
C	34.01065299942390	-27.40030136107517	2.79855657352016
N	36.18539786027468	-27.65712740726005	6.37871712947783
Fe	34.61763219087000	-26.59403791788252	5.65891342104204
C	34.13944712362197	-31.39963599366958	7.15443688134772
C	35.30853707283693	-31.93649706527929	6.34189289270212
C	31.99117265810748	-27.55524487718154	6.95107096039442
C	33.31932365814938	-27.89438527155209	6.31901429504772
C	33.41638547794533	-29.35377464120532	6.14163491678341
O	32.91264488804491	-30.00568211401190	5.24714063719786
O	34.10441320046779	-29.96514096272353	7.16897347468552
H	29.88562552633246	-22.44554261948045	4.14141127214391
H	31.16707925988538	-21.74734841495426	5.13913985177804
H	29.99918233808802	-22.85808768241307	5.85608807687320

H	31.33500321426573	-24.17498600210938	1.33970108596731
H	30.16708046211714	-25.33938530117623	1.96635900519816
H	29.96690159678707	-23.61647631944789	2.31005685089571
H	33.79276668827810	-27.36008366032237	-0.14252405263844
H	34.33385366014564	-29.03516915927209	-0.30285108829597
H	32.76220771236493	-28.67709823129163	0.42378609753258
H	36.09248213576557	-30.08257256668069	0.42765747952426
H	37.45192661285179	-29.68057521484283	1.48335287863082
H	36.32122879153412	-30.95371171264948	1.94850948176216
H	33.55134986008510	-22.65872651050692	10.68405205104904
H	32.11616167088324	-23.01127367333608	9.71363946682403
H	33.34253029768414	-21.90194312620828	9.09961335925660
H	36.60885211993698	-24.55567960804347	10.85425289801209
H	35.39337444284109	-25.68287361542192	11.45602173489830
H	39.48137630410236	-29.32501997311984	8.89504107775918
H	39.12351645992526	-27.65124855581776	9.33979715897662
H	38.05835357351449	-28.95255666047827	9.87518977950095
H	38.62535110537348	-31.00783462625343	5.81975126721664
H	39.65406293217104	-29.67336544125872	5.29664697765460
H	39.76455976747098	-30.27590724428802	6.95536127485851
H	35.09200836431826	-23.94213477995770	11.52592293715210
H	36.25060394773675	-31.52291896460308	6.70916319071248
H	35.35179337785588	-33.03045857218727	6.41221060288188
H	35.19857468115287	-31.65715595521355	5.29311487375790
H	33.19272481364357	-31.77907882590658	6.76187329558917
H	34.23069596851652	-31.68581240373094	8.20636983976018
H	31.85721467243153	-26.48506333775197	7.09599834691179
H	31.16001997942633	-27.92142535501122	6.32693576761321
H	31.87727532033687	-28.04624598706789	7.93240592516624
H	32.42583012122840	-26.46859367891569	1.75038663854701
H	36.77231407323167	-26.74474522511241	9.58531601604990
H	37.43848662305903	-29.69207183612485	3.98298443930152
H	32.16956513272771	-23.07814611241660	7.14087079551142
O	35.86482579547548	-25.34232069898363	5.00060646299241
H	35.52433757848455	-24.45488261589259	5.18700314507316

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B3LYP Scan/Hydroxide IPC Model/BSS/90 degrees Constrained Optimization

C	30.72266395224856	-24.36493638299679	2.19175890292871
C	35.50755539025128	-24.79499327662071	10.90366439836931
C	39.03550061949490	-30.08402678964064	6.09361980937344
C	33.81000673108849	-28.28122097753700	0.30865867829832
N	33.12141677984452	-25.42591793338782	4.87884378259740
N	34.49459048804992	-25.54123244842964	7.36757920937437
N	34.79543366638804	-27.55736017360208	3.85668594770869
C	32.96846110560629	-26.45137205067815	2.65986443622579
C	32.73866303741210	-23.94010125473857	6.78535023874632
C	36.24991110926813	-26.72513116183162	8.60036094210771
C	36.73678298923490	-28.95519389996434	4.34443971187237
C	30.58979720891491	-22.65385092718296	4.95532186803720
C	33.17682389954720	-22.88644600105266	9.67323235351053
C	38.65652171313218	-28.63750665936882	8.98753964583742
C	36.37756430107352	-29.93605200936388	1.42174611845281
C	32.57300309667357	-25.53743438784899	3.63356365412259
C	33.67267531363740	-24.49073286073308	7.66127282809969
C	36.69937915889543	-27.57902108236424	7.59703119027837
C	35.72967177870301	-28.48433937240219	3.50789488872491
C	31.53222034911157	-24.53509448678969	3.44352692961248
C	33.90325931909405	-24.02670196854098	9.02223704589846
C	37.84087111572423	-28.47674831080184	7.73842235238344
C	35.53238691443551	-28.91872332419736	2.12933218217975
C	31.47768525116093	-23.81129910438927	4.60447452882182
C	34.88341520818393	-24.83065306746467	9.53986931969064
C	37.99961726750981	-29.08792167328176	6.52442172046207
C	34.45240988336170	-28.22400429396846	1.66239673644355
C	32.48013753369727	-24.38595841953385	5.49067824821067
C	35.24560181026179	-25.76757289064736	8.48479965893292
C	36.94113905646738	-28.56774814150400	5.66619633581172

C	34.01284474903107	-27.36618689714750	2.75845881086795
N	36.17728041139858	-27.66573467851725	6.34136720640866
Fe	34.61168943378782	-26.59370550631097	5.62784629242454
C	34.11589010472208	-31.36865408894054	7.29648120587014
C	35.39720498542437	-31.87712824510898	6.65162275712975
C	31.99995219304678	-27.59158011347482	6.92988493902628
C	33.32351196213561	-27.90794449488042	6.27872389705532
C	33.47871619895754	-29.36693696577424	6.14262639553990
O	33.13426784364148	-30.05327224069627	5.20085295067690
O	34.02957474850604	-29.93674741281757	7.27401372527923
H	29.88640009018642	-22.42453649170522	4.14692100119144
H	31.16643820066768	-21.73940042990369	5.15532115641974
H	29.99521639482859	-22.85622609037589	5.85722935111685
H	31.35316063632311	-24.10415997009529	1.32981064970498
H	30.18597695006786	-25.28588038899310	1.92461500554132
H	29.97536478307551	-23.57105847133903	2.30061416483897
H	33.80864021127977	-27.29899016525209	-0.18472071775063
H	34.33310647154624	-28.97842167909043	-0.35510949615473
H	32.76277266902003	-28.60935290579794	0.36863352723405
H	36.08376564565001	-30.04264654362258	0.37150722566519
H	37.44186769475229	-29.66321859894680	1.43713062297758
H	36.29621487504659	-30.92910715622649	1.88592075774855
H	33.52330043400599	-22.72214555853235	10.69966870602559
H	32.09304569185809	-23.06453302669305	9.71852368604083
H	33.31966520361828	-21.94451939760325	9.12481067258320
H	36.58995898071986	-24.61157121242431	10.85182778822641
H	35.37356306533384	-25.74584027129491	11.43837597321737
H	39.46563623068067	-29.36305060381151	8.84821142863839
H	39.11619990998972	-27.68961382921505	9.30111636811433
H	38.04507848951980	-28.98819439914778	9.83094224678000
H	38.58336331142701	-31.03634970827359	5.78282035253296
H	39.62029290851763	-29.71562982679512	5.23920709641601
H	39.74213975106655	-30.30759513385684	6.90102103181637
H	35.07121059280723	-24.00610809527522	11.52638872195122
H	36.27047354377056	-31.41998234851524	7.12264044100722
H	35.46956394014751	-32.96697210179177	6.75447785498581
H	35.41122049695493	-31.62398419615320	5.59076817442968
H	33.24066460021628	-31.79044950570433	6.79587300544245
H	34.08215562705652	-31.63234037231152	8.35777569729232
H	31.84254291950108	-26.52219047111480	7.05788890426557
H	31.16340866085320	-27.98647397910341	6.32952602527205
H	31.91873127720162	-28.06861782286151	7.92061597279141
H	32.43571431687660	-26.41766407052408	1.71376406055741
H	36.76373722044804	-26.78049705227343	9.55592048250174
H	37.42058133655992	-29.69167839156632	3.93253611237592
H	32.15302700892853	-23.10040860793258	7.14831379672087
O	35.85921477319524	-25.33436472143754	4.98526234297177
H	35.51468038517707	-24.44896075690679	5.17397374811765

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B3LYP Scan/Hydroxide IPC Model/BSS/100 degrees Constrained Optimization

C	30.70109347042877	-24.38903120199639	2.19779031092704
C	35.51908135656208	-24.79058646869159	10.89272765728168
C	39.03007700294526	-30.09676510333588	6.08943599932768
C	33.83651915114758	-28.25674135049393	0.29008133046724
N	33.12340516958562	-25.42669614353954	4.87220240470085
N	34.50286224415559	-25.53808801028778	7.35769352099002
N	34.81035500425308	-27.54433595634538	3.84378441576787
C	32.97597012947568	-26.44729773757678	2.65081858341204
C	32.73705675973032	-23.94537097460296	6.78124352169083
C	36.25804850486300	-26.72256789560291	8.59104477528069
C	36.75094772808144	-28.94356766422944	4.33128213113148
C	30.56134341792436	-22.68383957711071	4.96466970296832
C	33.18200493849218	-22.88709806276567	9.66641967391461
C	38.65748387508629	-28.64450541356328	8.98120325754652
C	36.41002999274042	-29.90338284249140	1.40149524089934
C	32.57209043189025	-25.54151941301274	3.62865054234740
C	33.67859970015884	-24.48947924781453	7.65318566400032

C	36.70537225787428	-27.57884762351392	7.58878791608482
C	35.74868617828734	-28.46609767540043	3.49304061212456
C	31.51924444245227	-24.55081495733416	3.44510906959749
C	33.91066356479219	-24.02487808967924	9.01359067745493
C	37.84325658372293	-28.48084702966213	7.73144734509276
C	35.55771025134333	-28.89380468776221	2.11149287381571
C	31.46176793668403	-23.82956401216845	4.60758590491813
C	34.89319766653471	-24.82696563985093	9.52973382526549
C	38.00138472450178	-29.09224761432288	6.51737101485572
C	34.47535264720035	-28.20259205991906	1.64558335498346
C	32.47453981076798	-24.39442032316155	5.48838098172384
C	35.25523609162992	-25.76348744018717	8.47444786276815
C	36.94810266052242	-28.56611003012502	5.65693850826076
C	34.02864826130921	-27.35287400882499	2.74533642840072
N	36.18433016563574	-27.66369358296053	6.33227200694115
Fe	34.61959243054199	-26.58783260647225	5.61576366399463
C	34.00686940567581	-31.39319494010466	7.27061559306340
C	35.35077507379713	-31.86917816011367	6.73627774557539
C	32.04724020213334	-27.58934143444408	6.99439075884928
C	33.33042020793266	-27.90574905752759	6.26721610775212
C	33.48416177528009	-29.36103021559486	6.10890870567216
O	33.24645609844741	-30.02471293244400	5.11962688636553
O	33.90482942157826	-29.96280091739671	7.28310620279400
H	29.85285949358293	-22.46054564667343	4.15901445105606
H	31.12756831222162	-21.76312952787342	5.16564061046888
H	29.97180715737571	-22.89586282766123	5.86770508694349
H	31.32297178111415	-24.11517060050739	1.33360783276717
H	30.17786478093937	-25.31750940365056	1.93009912934096
H	29.94176317032804	-23.60759005448296	2.31317354153746
H	33.82985578374615	-27.27202828493370	-0.19827315868832
H	34.36584710184123	-28.94704199017811	-0.37599011987516
H	32.79138989764765	-28.59232416451525	0.34572360138913
H	36.11985476904933	-30.00653856919778	0.34989782321647
H	37.47289306738466	-29.62520720814281	1.42130345688853
H	36.33217670002535	-30.89887151246957	1.86099720969347
H	33.53135403704005	-22.72094175571126	10.69157680353174
H	32.09912121371556	-23.06963507737720	9.71559659182946
H	33.31908720434163	-21.94494723911088	9.11697836936089
H	36.60100635043314	-24.60470481917345	10.83954031816123
H	35.38796786115543	-25.74205557870039	11.42702847692230
H	39.46635346712458	-29.37016905802880	8.84110061634804
H	39.11754144155429	-27.69738266411311	9.29654462268215
H	38.04553945112718	-28.99625820194797	9.82378415664802
H	38.57050251237644	-31.04785489485903	5.78579698707152
H	39.61463668641581	-29.73730336933778	5.23108486848460
H	39.73771407992478	-30.32002530341035	6.89602633206726
H	35.08175356710511	-24.00309952628507	11.51650967962993
H	36.17114892594282	-31.41302560277646	7.29567192035977
H	35.43034103133466	-32.96018135904455	6.82023254965798
H	35.45892273978887	-31.59066446320009	5.68738960366986
H	33.18968116486863	-31.80843255621685	6.67511256018448
H	33.87449649925234	-31.69070125486302	8.31518770017746
H	31.90054417611425	-26.52049119886777	7.13774083859823
H	31.17367897456455	-27.97627797914311	6.44277900091432
H	32.02441966245699	-28.07399918839959	7.98353171838404
H	32.44235522179019	-26.41480930394177	1.70516388526390
H	36.77168229985310	-26.77805100429070	9.54668614800252
H	37.43611890593987	-29.67793970404273	3.91790193089147
H	32.14710858020036	-23.10983243427161	7.14677409582731
O	35.86332650504440	-25.32505363113753	4.97466378116509
H	35.53613266674863	-24.44230526603109	5.20272998342011

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B3LYP Scan/Hydroxide IPC Model/BSS/110 degrees Constrained Optimization

C	30.67881093152775	-24.41192959082947	2.20467425089735
C	35.53031608889000	-24.77900859359089	10.88204172836937
C	39.03047723732914	-30.09891992454421	6.08528093280077
C	33.84895305812451	-28.24474402287735	0.28029370612856

N 33.12224980558920	-25.42812463359902	4.86776710349572
N 34.51067122586873	-25.53159516313778	7.34883876428342
N 34.82538396435231	-27.52781745298247	3.83228866682629
C 32.97698127304368	-26.44753259160673	2.64615844989391
C 32.73637235043737	-23.94639940204831	6.77645783182468
C 36.26567030447694	-26.71574700201169	8.58306387878821
C 36.76982317385760	-28.92264670593854	4.31736037707642
C 30.53916297518424	-22.70570719755245	4.97073881018650
C 33.18995688172600	-22.87924505672658	9.65652297681075
C 38.65572693280449	-28.64894932753948	8.97764548818429
C 36.43588238623546	-29.87451856985830	1.38583985224529
C 32.56675486597955	-25.54757568802468	3.62667904036315
C 33.68484554841805	-24.48392077870838	7.64485406253308
C 36.71310732516507	-27.57225373505507	7.58093455812506
C 35.76882347371605	-28.44301901088722	3.47918193143155
C 31.50460583012280	-24.56615007698835	3.44796228704415
C 33.91886302019537	-24.01708738565282	9.00398068650511
C 37.84719038289421	-28.47849035675499	7.72507826523666
C 35.57910157351156	-28.86982075469644	2.09718235918150
C 31.44703546271224	-23.84448557849644	4.61029860375757
C 34.90275942489591	-24.81780738813505	9.51986291664435
C 38.00742280405683	-29.08748693978919	6.50997580374301
C 34.49083894908144	-28.18640235934558	1.63415920312983
C 32.46865048867067	-24.40051933943888	5.48640610348972
C 35.26407070751184	-25.75540553302843	8.46540005609938
C 36.96073692112385	-28.55406506796777	5.64633005425610
C 34.03974642082984	-27.34166412203428	2.73610046035804
N 36.19594388065980	-27.65262290772266	6.32229532165735
Fe 34.62916310152063	-26.57891415839370	5.60482958980172
C 33.90344728702467	-31.42804854482581	7.23456430546276
C 35.29226683563104	-31.88714994640037	6.80992333342649
C 32.10313691587781	-27.59579071279088	7.05608849760077
C 33.34621402927205	-27.91055465303248	6.26150573864051
C 33.50751337316881	-29.36076822476860	6.08184486392142
O 33.38733887952856	-30.00125718033581	5.05662490064186
O 33.79433016671727	-29.99978935610925	7.28125372805320
H 29.82553847279511	-22.48845021387253	4.16795822199253
H 31.09899353967009	-21.78042167071348	5.16859925533620
H 29.95509272598004	-22.92156901804913	5.87641883392684
H 31.29318632231470	-24.12891702065791	1.33805694620939
H 30.16550995060931	-25.34611757301582	1.93772002839639
H 29.91069871777141	-23.63988435689586	2.32514819132157
H 33.83151313086841	-27.25952702069677	-0.20677165642207
H 34.38314506503858	-28.92908436715457	-0.38805534023675
H 32.80725510970733	-28.59055629334756	0.33816014778191
H 36.14558012504617	-29.97832286411110	0.33433108251835
H 37.49745648347123	-29.59146820879928	1.40537816109912
H 36.36248578191422	-30.87047525451096	1.84504224402882
H 33.54241770771236	-22.70984294129237	10.68007432852951
H 32.10763130555335	-23.06397014994714	9.70985027778621
H 33.32315790025510	-21.93821120182735	9.10425319568487
H 36.61204297357276	-24.59249418511235	10.82728896149001
H 35.40039882842548	-25.72974674759187	11.41791507213859
H 39.46370717279457	-29.37566025502283	8.83801330369698
H 39.11643165812185	-27.70400526256663	9.29857622424958
H 38.03968678726717	-29.00269726045441	9.81638834063211
H 38.56516964061474	-31.04810666178213	5.78455545507619
H 39.61737991721137	-29.74570223539004	5.22596481895077
H 39.73652043843887	-30.32385125056323	6.89276689620436
H 35.09315809612981	-23.99090066447499	11.50515480514840
H 36.05844290786287	-31.44634546816167	7.45256228790389
H 35.36908754632470	-32.97991280711652	6.86964196334147
H 35.49032981182246	-31.578163329952590	5.78311632203876
H 33.14642437782087	-31.82647342946762	6.55383260599075
H 33.67642672997234	-31.75844070270465	8.25274443013188
H 31.95534445485250	-26.52623889828379	7.19186687756804
H 31.20043310259794	-27.99674679387710	6.56453012595583
H 32.14370832673217	-28.06523977857677	8.05109630836838

H	32.44020291046350	-26.41918970684008	1.70215872253685
H	36.77801867444214	-26.77222390894202	9.53932856583610
H	37.45644740533471	-29.65482773087762	3.90254155879135
H	32.14380587073148	-23.11327764953780	7.14324993137296
O	35.86281408307936	-25.30839164816873	4.96338006323070
H	35.54820366694550	-24.43053079284303	5.22565873547731

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B3LYP Scan/Hydroxide IPC Model/BSS/120 degrees Constrained Optimization

C	30.66426715902535	-24.42336212388633	2.21120999230803
C	35.54139767930428	-24.79752811289932	10.87330658056993
C	39.06675083382149	-30.06909689489335	6.04539516759827
C	33.85945219067366	-28.22382838100226	0.25972570878394
N	33.12669883712658	-25.43007715674738	4.86002980921826
N	34.51640841707699	-25.54148314995326	7.33965430798518
N	34.83993428763749	-27.51423315885305	3.81184149655954
C	32.98019846733602	-26.44297214513716	2.63569775262575
C	32.73840613105443	-23.95750157306672	6.77561238129319
C	36.27651898044238	-26.72533308665948	8.56708926962219
C	36.79195213923536	-28.90202132171796	4.28730455568912
C	30.52647858752069	-22.72518807310888	4.98244689931057
C	33.19579121130956	-22.89807268829085	9.65775351602169
C	38.68389974416026	-28.63909213882690	8.94596362775146
C	36.46072268813644	-29.83971380430025	1.35290537780711
C	32.56711756621444	-25.54929115207626	3.62074226486162
C	33.68960345451308	-24.49577813364020	7.64032841039954
C	36.72722895455998	-27.57451154666034	7.55998209840780
C	35.78832009463551	-28.42171069670696	3.45316373811752
C	31.49772298430334	-24.57463119067573	3.44972956357035
C	33.92512035084976	-24.03289307468359	9.00044916711030
C	37.86955152389888	-28.47133528927507	7.69673220680862
C	35.59882251014390	-28.84339465223107	2.06964520677629
C	31.44073092780805	-23.85636246113739	4.61432935348103
C	34.91085785551835	-24.83391506158193	9.51241749365061
C	38.03301775952068	-29.07180489569217	6.47782670369246
C	34.50440108816297	-28.16637343913805	1.61214178047875
C	32.46929609445379	-24.40848085509127	5.48457947972724
C	35.27189910529925	-25.76760798063896	8.45445845542767
C	36.97961888120574	-28.54370054524158	5.61929512721571
C	34.05013780735419	-27.32934319006774	2.71882875975321
N	36.20782306252767	-27.65284636653884	6.30202624197940
Fe	34.63796990372453	-26.57919337670663	5.58892711572751
C	33.75323920767878	-31.45510015655024	7.22942751009377
C	35.19664582970301	-31.89785626625468	7.02638300650640
C	32.13494056054497	-27.59752352259962	7.07215105631589
C	33.35205523325897	-27.92131624294671	6.24059047769032
C	33.51906632909752	-29.36832915423054	6.06078388886625
O	33.53696919360493	-29.99818435018943	5.02169898725693
O	33.63063083170053	-30.02995470832185	7.28249705049873
H	29.80824069422902	-22.50994676461074	4.18325349534026
H	31.08070948777292	-21.79678057296982	5.18145166706128
H	29.94739997144709	-22.94819524029597	5.88960698386770
H	31.27117864833293	-24.13066566625838	1.34255654429920
H	30.15889483143378	-25.36153186903651	1.94314532621387
H	29.88910156130723	-23.65957067110997	2.33890047072600
H	33.83639201062088	-27.23745458073013	-0.22482203714330
H	34.39507990010673	-28.90401965584591	-0.41170876544093
H	32.81943091685632	-28.57444878521197	0.31911413730915
H	36.16620489284870	-29.94506484629775	0.30272386931240
H	37.51997424414856	-29.54765538394120	1.36761569189331
H	36.39773782378356	-30.83636396298705	1.81199910560955
H	33.55006632523796	-22.73104533535747	10.68107418293436
H	32.11388817837899	-23.08473615307046	9.71282223120290
H	33.32632495016266	-21.95522316864019	9.10797666164043
H	36.62254114443530	-24.60817143243841	10.81654028562492
H	35.41512254336569	-25.75002915348105	11.40688953165768
H	39.49298269695295	-29.36398170518047	8.80341173961782
H	39.14397803944809	-27.69282801588117	9.26407925703121

H	38.07262726630020	-28.99340689563889	9.78790978024554
H	38.61230629326737	-31.01954884352491	5.73251734333888
H	39.65292215044051	-29.70051344559701	5.19201074727601
H	39.77237676658717	-30.29601459383873	6.85263826234419
H	35.10383594582462	-24.01221302327654	11.49965219449049
H	35.84554626228505	-31.46035904422114	7.78954216460007
H	35.27598681840912	-32.99059206831564	7.08249540842442
H	35.55474547639144	-31.57230210436065	6.04883962084757
H	33.11918064848109	-31.84457931575232	6.42877568602083
H	33.36782465031787	-31.80670707369861	8.19164090978475
H	31.93726567999209	-26.52840358542524	7.11481085190152
H	31.22823822587226	-28.09206084963329	6.68582236203162
H	32.26260843478717	-27.96070489135683	8.10307688345862
H	32.43992130388799	-26.41531179626319	1.69367505413165
H	36.79095752082967	-26.78336561791128	9.52211855259941
H	37.48283744657914	-29.62689324524599	3.86680169501855
H	32.14357309547120	-23.12795774224832	7.14674651768535
O	35.86756229404050	-25.30280828271389	4.95527854547585
H	35.55696437322268	-24.42752282641284	5.23073123700878

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B3LYP Scan/Hydroxide IPC Model/BSS/130 degrees Constrained Optimization

C	30.67847181596780	-24.36436427911001	2.19219489431568
C	35.50843284072252	-24.93762725919117	10.86855127077859
C	39.08903098345593	-30.06076796219823	5.91897953297071
C	33.85754673719553	-28.14802491260141	0.18165758737191
N	33.13004614302454	-25.43195982765735	4.82802875762905
N	34.50835020644848	-25.59590362716131	7.31150628775768
N	34.83034766425109	-27.50780450153023	3.74906988097127
C	32.97423924880823	-26.41172679645921	2.58923702816983
C	32.74102659511077	-23.99281347346241	6.76955835282503
C	36.26644032327493	-26.80366503164089	8.51852277068994
C	36.79734842145097	-28.88447252030358	4.19313279619940
C	30.55195887900621	-22.70695351830222	4.98829356094082
C	33.17288917042615	-23.00798416388219	9.68136262601135
C	38.69697131472085	-28.69851181301535	8.85112289688247
C	36.46601747605065	-29.77299174302086	1.24455400527070
C	32.56950761297094	-25.52823326005607	3.58666778788713
C	33.68069022474683	-24.55718089977643	7.63029121451300
C	36.72563960386265	-27.62575699452422	7.49245345868389
C	35.78530907352125	-28.40126639202679	3.37236730770350
C	31.50873382696492	-24.54208153081397	3.42928979484938
C	33.90672136414020	-24.12714676497786	9.00264073979342
C	37.87789523269688	-28.51290671094932	7.60764776985105
C	35.59744535860303	-28.79729816568251	1.98145352426905
C	31.45670540592042	-23.84055116609344	4.60429667335235
C	34.88845257923470	-24.94076564142442	9.50245578233987
C	38.04480385386437	-29.08539434090051	6.37591720007064
C	34.49887275798718	-28.11757148220756	1.53680171965421
C	32.47868179169325	-24.41473905696764	5.46762389642709
C	35.25760008431067	-25.84833169526766	8.42488993554482
C	36.98410222102211	-28.55047542327157	5.53072442443148
C	34.04112818162214	-27.30355992222126	2.65897946960128
N	36.20448628477724	-27.68253364168968	6.23391122551733
Fe	34.63433357465079	-26.60012946661685	5.54311552020316
C	33.71592142559565	-31.38753167589078	7.49786180577173
C	35.19668040081726	-31.71706070879057	7.63917522069935
C	32.07815479257226	-27.61234954598135	6.93998967027363
C	33.34892407475508	-27.95155912833699	6.20019613743741
C	33.60700259793207	-29.39325372817967	6.15979038657689
O	33.87730689053288	-30.08489751896023	5.19728774158890
O	33.48720118117530	-29.97804571457810	7.42460029235631
H	29.83468787646494	-22.47555163064152	4.19280931100885
H	31.11400200730508	-21.78578774468707	5.19873927448962
H	29.97219173169491	-22.93723980587636	5.89313739073912
H	31.28760798277361	-24.05458715508076	1.33099210059343
H	30.17250182750163	-25.29611019764442	1.90377327862419
H	29.90386785904460	-23.60246529795473	2.33377467468693

H	33.84112669621991	-27.15312634147858	-0.28555705186986
H	34.39189652385260	-28.81883439391784	-0.50014800576400
H	32.81536486651469	-28.49393207757693	0.23085061416284
H	36.16781553657035	-29.86420476878189	0.19406226999694
H	37.52222273269187	-29.47013608968680	1.25929559004051
H	36.41543243018204	-30.77727237060845	1.68798550331025
H	33.51511733476237	-22.86942515370664	10.71298738550629
H	32.08997590090551	-23.19286108785828	9.71841128158106
H	33.31259528592969	-22.05103008644613	9.15885152506082
H	36.59071145139939	-24.75155327225251	10.82420455568130
H	35.37409039639936	-25.90122378878401	11.37979496369799
H	39.51270142214544	-29.41231054008071	8.69162112726966
H	39.14857798797357	-27.75450764250491	9.18748954697626
H	38.09173947326399	-29.07618174753216	9.68730437917295
H	38.64394453273260	-31.00520216644759	5.57625070407589
H	39.67486117515203	-29.66187970491615	5.07906300188033
H	39.79331997279872	-30.30523447161686	6.72213623289720
H	35.06940047621252	-24.16452416863374	11.50890313480443
H	35.62648596338973	-31.20319670604719	8.50314989749933
H	35.34149505680414	-32.79694516047767	7.76714510472178
H	35.73880197718885	-31.39553976608691	6.74911725935348
H	33.30236178760049	-31.86984289585106	6.60848011658027
H	33.15505892404338	-31.72050307143098	8.37697129049590
H	31.82220908424618	-26.55823526974904	6.85588475947205
H	31.21824769189412	-28.19859739474861	6.57738680349736
H	32.17730363501344	-27.85188501141953	8.00885407842396
H	32.43441357747010	-26.36653363803607	1.64764136081229
H	36.77926657539768	-26.88042136843885	9.47306172002295
H	37.49218656052609	-29.59668091406595	3.75804808387925
H	32.14807514610710	-23.16823131466605	7.15436948208920
O	35.87033628472524	-25.31975935032323	4.93449482573428
H	35.52078001721713	-24.44217475522178	5.14924726361358

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B3LYP Scan/Hydroxide IPC Model/BSS/140 degrees Constrained Optimization

C	30.65997083225422	-24.40754445197187	2.20954130419501
C	35.53236175916582	-24.93414213049908	10.86438121516994
C	39.11869235256965	-30.04982393137163	5.90730605500867
C	33.88970358805948	-28.13397098706979	0.17318031516999
N	33.14104458528516	-25.44277356812602	4.83026601748204
N	34.53546417044183	-25.59080388595660	7.30611686896190
N	34.85585175206735	-27.50077429314246	3.74399500512696
C	32.98508371246593	-26.42310873718137	2.59169175845315
C	32.74827928074017	-24.00659001740367	6.77314781876172
C	36.29722108815145	-26.79503796124957	8.51157111289757
C	36.83536842991648	-28.86137358525092	4.18085169928766
C	30.53099727466997	-22.74915433956736	5.00480232183963
C	33.18019306237048	-23.02067231649163	9.68401669976882
C	38.72302041107946	-28.69709989648240	8.84398785375150
C	36.51856040757640	-29.73200229907630	1.22676873155560
C	32.57431349461525	-25.54619888976920	3.59235835432276
C	33.69890752519947	-24.56003883159348	7.62848974144998
C	36.75682150019720	-27.61597826340258	7.48476381475086
C	35.82073801786339	-28.38113873123422	3.36225032717407
C	31.50023046796590	-24.57392283112107	3.44160574070254
C	33.92323874601400	-24.13139362378050	9.00133569626444
C	37.90778020603241	-28.50487570501494	7.59911241087815
C	35.63765951784956	-28.77159106648666	1.96914191622171
C	31.44717985490109	-23.87208442679539	4.61653095628522
C	34.91184454658202	-24.93859254332192	9.49848611575228
C	38.07598955277206	-29.07352960119256	6.36576181952611
C	34.53045410270798	-28.10346701144575	1.52861014285593
C	32.48185798079607	-24.43278838031248	5.47353383719399
C	35.28668928776986	-25.84113866857333	8.41883778208155
C	37.01718501142083	-28.53498600502080	5.52063054200476
C	34.06361917068612	-27.30099379884861	2.65551107357211
N	36.23638073300287	-27.67019819533129	6.22571696905642
Fe	34.65997076834923	-26.59544996768882	5.53876664546464

C	33.52627028533904	-31.45056339175827	7.40081186291039
C	34.97297095058427	-31.82254582898678	7.70417869376316
C	32.16620562221501	-27.58956463219291	7.03724211492909
C	33.38140367936271	-27.95750729181015	6.21969104565323
C	33.61109430233545	-29.39945595117862	6.14485551434737
O	33.97220674787523	-30.06293938928128	5.19106557906752
O	33.33522181438529	-30.03518642082684	7.36394767931141
H	29.80050017992832	-22.53365683162806	4.21690864443894
H	31.08211750063032	-21.81841711767149	5.20172514743492
H	29.96622135698180	-22.98152460088109	5.91846936143839
H	31.25506352860980	-24.06637223419429	1.35026407656096
H	30.18438485980827	-25.35179903083929	1.91085734897371
H	29.86106643425260	-23.67369266045759	2.36376614034141
H	33.85630725418294	-27.13567795066012	-0.28567404415580
H	34.43579652415539	-28.78977992515696	-0.51392085941644
H	32.85364443400574	-28.49834580171678	0.21899027080789
H	36.22354223889237	-29.81872246924014	0.17499797363485
H	37.57112703440790	-29.41708921125250	1.24614351631306
H	36.47858092735280	-30.74009260983393	1.66260536519771
H	33.52032882154711	-22.88367121137939	10.71652325303170
H	32.09881953066380	-23.21448617801606	9.71925767247657
H	33.31266253412090	-22.06050267985606	9.16557209326528
H	36.61256155707041	-24.73618584238814	10.82046752651669
H	35.40852885370946	-25.90114708860535	11.37177015852745
H	39.54435297138571	-29.40361696843805	8.68091687831074
H	39.16662053278603	-27.75334432979789	9.19137758462218
H	38.11663115177640	-29.08715226701194	9.67365196666552
H	38.67142853907834	-30.99227682500013	5.56205967281639
H	39.70574202565189	-29.65018733638415	5.06857590078826
H	39.82214143245439	-30.29740371143393	6.71024641158719
H	35.08521962089161	-24.16841545952740	11.50792837934904
H	35.30479620401296	-31.35337061763282	8.63459714314808
H	35.08014900081218	-32.90963426410573	7.80529651172215
H	35.62566452726067	-31.48189516666421	6.89911649077717
H	33.21444944626135	-31.88567623936238	6.44792424864034
H	32.85821697619433	-31.80756652562540	8.19128922632159
H	31.78891550219316	-26.60215095809043	6.77417418693890
H	31.34518681019510	-28.31369773967568	6.94065341309649
H	32.42085720220771	-27.55862973336284	8.10751086161195
H	32.44123634837799	-26.38239669112413	1.65225302194246
H	36.80985320808935	-26.87241144619314	9.46617827583650
H	37.53468542819098	-29.56749883515352	3.74309065941130
H	32.14825092471935	-23.18870767276124	7.16122447728211
O	35.88301519542963	-25.30881619090828	4.92163582647389
H	35.54819594107450	-24.43456927316037	5.17101340630069

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B3LYP Scan/Hydroxide IPC Model/BSS/150 degrees Constrained Optimization

C	30.63968335068864	-24.42546401642127	2.22021536582969
C	35.52198965983418	-24.98589201888592	10.86479221881727
C	39.15777863980511	-30.01394480517030	5.85264237747405
C	33.88703784219683	-28.12168130462324	0.15353690003513
N	33.14679887909595	-25.44731917499547	4.82120694417017
N	34.54571919122046	-25.60346908851690	7.29426234400626
N	34.87126093890664	-27.48506306014627	3.71886634332491
C	32.97773177099727	-26.42882169075373	2.58396622416622
C	32.75854089328949	-24.01645759629717	6.76910918399098
C	36.30147102522287	-26.82052683906402	8.49515427669015
C	36.87783171687707	-28.81152681821433	4.13461570385083
C	30.52991779302220	-22.76140506136632	5.01328395258336
C	33.18023141041966	-23.05616770291803	9.69025007047638
C	38.72979410977561	-28.72281955500966	8.81354930368651
C	36.55616045873050	-29.67172950913718	1.17785921372059
C	32.56991044605916	-25.55441813702936	3.58817883758378
C	33.70801509976812	-24.57550358119041	7.62225671346986
C	36.77072674468661	-27.62357019183499	7.45841674321928
C	35.85070629628500	-28.34378990510073	3.32492824558356
C	31.49111649935991	-24.58642126628246	3.44531247473792

C	33.92596661368378	-24.16052324475729	9.00024844062706
C	37.92526562395218	-28.50936110989541	7.56527603901338
C	35.66374619871326	-28.73093736774712	1.93160877632400
C	31.44615587837809	-23.88229959841765	4.61935749607989
C	34.91013840866515	-24.97477380257008	9.49507706271507
C	38.10732993511151	-29.05126742647985	6.32189849547295
C	34.53910141880696	-28.08358781529697	1.50343928876851
C	32.48875052461933	-24.43913349179940	5.46900793065339
C	35.29066908877206	-25.86612354909180	8.40828144220711
C	37.05158880818085	-28.50286739503138	5.47912305740149
C	34.06731223992136	-27.29387428248116	2.63718120351637
N	36.26059931951220	-27.65693918350319	6.19465293224826
Fe	34.67597598939145	-26.59262123577113	5.52010725749953
C	33.45946352202884	-31.46781235020602	7.39096580542951
C	34.82608144397962	-31.76448130253856	7.99841989391320
C	32.17750769679134	-27.60122306912655	7.00041782042938
C	33.40700262984357	-27.97069949000752	6.20709525793248
C	33.67100788781969	-29.40595394531553	6.16519534600413
O	34.21144502782339	-30.05246475920519	5.28643949846657
O	33.20965644077653	-30.06444016013255	7.31890901301422
H	29.79357868489813	-22.54807498253299	4.23026911175272
H	31.08031859881396	-21.82934495721734	5.20588010796610
H	29.97185109546423	-22.99439620131686	5.93089857225806
H	31.22645329589283	-24.08574917227439	1.35467577525520
H	30.16353779553142	-25.37166504879434	1.92858577669112
H	29.84048120803396	-23.69295016483204	2.37916456238721
H	33.83350919079207	-27.12320809229302	-0.30297463009245
H	34.43766877753541	-28.76716932804449	-0.53972324759366
H	32.85733072715723	-28.50268789765136	0.20734352570285
H	36.25070415097338	-29.76408160126007	0.12955258406952
H	37.60202742464561	-29.33475206931487	1.18538647090020
H	36.54266874946029	-30.68064483905250	1.61343732135809
H	33.51138350343839	-22.93344024482423	10.72746202998623
H	32.09805735162145	-23.24709211719057	9.71340980323947
H	33.32016640796751	-22.08979137436478	9.18544929997895
H	36.60263118992297	-24.78856312720477	10.82996459682774
H	35.39396985061126	-25.95824431589275	11.36083387839739
H	39.55434917617934	-29.42432789151180	8.64502757451671
H	39.16802609174894	-27.78473173780442	9.18250895674159
H	38.11648603817719	-29.12956158478123	9.62995175158328
H	38.71577088554502	-30.94894730859630	5.48170742322995
H	39.75247610676930	-29.59405550305385	5.02929506287775
H	39.85347013575012	-30.27783733870893	6.65715031250949
H	35.07152659426610	-24.22682845013980	11.51389344069673
H	34.91876155356886	-31.29572037130000	8.98247014208195
H	34.97421675216035	-32.84534540236679	8.11339103285982
H	35.61826451357845	-31.37270670015591	7.35797604054833
H	33.38500618357433	-31.90384855797525	6.39196513113597
H	32.65858626607868	-31.87283592574405	8.01844733542350
H	31.80377962039952	-26.61546172290509	6.72799118155058
H	31.36113130479397	-28.32818964790161	6.89489885978841
H	32.41419370232781	-27.56605954644319	8.07486682046817
H	32.42528877166787	-26.39281162901227	1.64936840106836
H	36.80772583832488	-26.91095444009337	9.45199439476931
H	37.58730607250362	-29.50207749783853	3.68846174523297
H	32.15810040484774	-23.20108512179181	7.16175577095472
O	35.88892540113006	-25.29525345724099	4.90997587289195
H	35.53799227383509	-24.42371227124120	5.14648105685222

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B3LYP Scan/Hydroxide IPC Model/BSS/160 degrees Constrained Optimization

C	30.60608533648718	-24.49631536861839	2.26183231826281
C	35.57683101036416	-24.93605150810665	10.86220018000754
C	39.25779057167144	-29.91001021749242	5.83299486275176
C	33.88005116243097	-28.16629950479559	0.18893706326869
N	33.15375721643501	-25.46707328261346	4.84300249124255
N	34.57439401496513	-25.59229064021407	7.30593265843433
N	34.89433622803993	-27.48773859504152	3.73793117683961

C	32.96646773445180	-26.47556387060311	2.61961732912073
C	32.77792533115625	-24.01601005810366	6.77875100984561
C	36.35299808336703	-26.78185990957754	8.49900125669743
C	36.94310647312187	-28.75449296412846	4.13258710762844
C	30.52305089842682	-22.79472885588845	5.03365033054322
C	33.21813719807218	-23.02715892437496	9.68813570445561
C	38.81801379243596	-28.63831803343031	8.80103975603103
C	36.60603613399181	-29.63564764944494	1.18237770064088
C	32.56174339811637	-25.59407541995288	3.61899957667516
C	33.73517429511080	-24.56430558565736	7.63053083149873
C	36.82974892651501	-27.57596406054096	7.45876048218672
C	35.89235403296672	-28.32050412040759	3.33443032154109
C	31.47498538202802	-24.63483992526944	3.47735298298244
C	33.96212945597470	-24.13563455927032	9.00282552713942
C	38.00391521192533	-28.43726095747434	7.55692323222958
C	35.69733902073419	-28.71807799735214	1.94536519490997
C	31.44154814793562	-23.91462918721711	4.64209447147327
C	34.95325081173008	-24.94142378244536	9.49770586341673
C	38.19186711405121	-28.96917481799651	6.31065651032758
C	34.54898279174327	-28.10409740125309	1.52980044161026
C	32.49768899430928	-24.45431593198741	5.48581187081969
C	35.33013980304590	-25.84011961342224	8.41592406691709
C	37.11908387275985	-28.44238151003759	5.47564348451633
C	34.07219655431804	-27.32078687242720	2.66555099918770
N	36.31330505565970	-27.61727946098526	6.19839144678906
Fe	34.70630783604015	-26.58807069749918	5.53548220234699
C	33.22403361525539	-31.53923914564343	7.22406220357445
C	34.47302340765669	-31.91596875593553	8.01369744282058
C	32.19138247234734	-27.62050965649088	6.97531989636777
C	33.45336549579343	-27.98462928387303	6.23369304086436
C	33.71474832059124	-29.42061356472383	6.19481710233220
O	34.42895754514518	-30.04136927809104	5.42660917505082
O	33.01631554770194	-30.12841854857975	7.19255852030242
H	29.78896172224367	-22.58146785322261	4.24851777135952
H	31.07224068692707	-21.86257698067816	5.22868053972555
H	29.96201514508403	-23.02858962234363	5.94937114867499
H	31.18499461226576	-24.19700298141217	1.37649236854589
H	30.10592080394418	-25.44142465623115	2.00878329686355
H	29.82449891788257	-23.74280250606233	2.40972604932992
H	33.79127510356607	-27.17146828164538	-0.26990852428588
H	34.44009087202245	-28.79778220008366	-0.50968860050214
H	32.86261666974446	-28.57681931222777	0.25765593742884
H	36.27934793994774	-29.75375069167118	0.14310949723135
H	37.63854530922384	-29.25997524482002	1.16054966024949
H	36.64075095885646	-30.63814115836597	1.63124618567559
H	33.56323776045108	-22.88764966319416	10.71866385627171
H	32.13766859965065	-23.22496222767512	9.72939154749109
H	33.34428662088989	-22.06708249232880	9.16795654991128
H	36.65558518899536	-24.73076717965833	10.81639856904418
H	35.46059026657745	-25.90504224293906	11.36764410926501
H	39.64984992689882	-29.33042327012120	8.62931008534189
H	39.24732487467423	-27.69435194723073	9.16575713298895
H	38.21400845957574	-29.05025112925503	9.62176719100491
H	38.83011254796495	-30.85100422011055	5.46043875702914
H	39.84086468698609	-29.47597922266133	5.00859843789133
H	39.96198774927543	-30.16441776497198	6.63318926722539
H	35.1260077379943	-24.17494898374987	11.50866760438652
H	34.42471254305085	-31.51009333166500	9.02864964006110
H	34.57493480378787	-33.00607476051601	8.08133559638177
H	35.36186435154338	-31.51503576552843	7.52398774389906
H	33.29457661272291	-31.92132149962888	6.20250584767926
H	32.32644198562048	-31.95075148528696	7.69737007869046
H	31.92050143899952	-26.57694312536156	6.83591760326551
H	31.33670702543524	-28.24437662843534	6.67780823687901
H	32.31577029896111	-27.78982416966359	8.05545497390948
H	32.40187617810330	-26.45666500367916	1.69176135272901
H	36.86749210959072	-26.86260983425813	9.45233479896189
H	37.66747872972002	-29.42501626634794	3.67979625964749

H	32.17752100405769	-23.19904384434831	7.16812865576246
O	35.89208630270740	-25.27458158865456	4.91038241574557
H	35.51759427637879	-24.40731488999904	5.12554986658916

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B3LYP Scan/Hydroxide IPC Model/BSS/170 degrees Constrained Optimization

C	30.57557765532093	-24.56935646532118	2.30052679371433
C	35.63256676244905	-24.85368393118435	10.85779817856409
C	39.32634067981429	-29.83349602257474	5.85076565095436
C	33.86566581624575	-28.23559545070060	0.24339235067297
N	33.15195860716022	-25.48774421685597	4.87180585777704
N	34.59755806542739	-25.56901035704315	7.32216390905045
N	34.91391160624890	-27.49070352007852	3.76897264254019
C	32.95464876604395	-26.52613042120873	2.66320486157078
C	32.78953816341220	-24.00804748411493	6.78824964154491
C	36.39305694509739	-26.73214137694622	8.51491891632718
C	36.99045682393322	-28.71442979093769	4.15426308667198
C	30.51063147638438	-22.82563103211213	5.04652321536713
C	33.26008929586698	-22.96715026311204	9.67550766972042
C	38.87649589523751	-28.56231692672762	8.81721649167786
C	36.63617325560013	-29.63356926688912	1.21670773602344
C	32.54968254320269	-25.63644516491591	3.65543161375188
C	33.75873419868872	-24.53779262142164	7.63849706252010
C	36.87210716892339	-27.52828356971798	7.47725240775622
C	35.92393737332617	-28.30740637025810	3.36247797679611
C	31.45573442532111	-24.68595913127893	3.51024640735859
C	33.99790690438488	-24.08668654163553	9.00156634463869
C	38.05834833998646	-28.37303800297573	7.57390913526570
C	35.71949345195291	-28.72462518137987	1.98051231354261
C	31.42979296937023	-23.94812090611637	4.66419874080478
C	34.99487060159783	-24.88304467193884	9.50006214934863
C	38.25054748437929	-28.90404162515455	6.32817765366861
C	34.55275646678539	-28.14012965748796	1.57312553105526
C	32.49681958345019	-24.46932210270958	5.50584215413873
C	35.36397602522719	-25.79751910235417	8.42883328441430
C	37.16739641762696	-28.39519240350080	5.49538722821347
C	34.07499567135748	-27.35240521671279	2.70546444239639
N	36.35161164101732	-27.58110166634673	6.21930547453725
Fe	34.72621872254624	-26.58064345956565	5.55940480371289
C	33.05317082546379	-31.59836974966333	6.96093774341622
C	34.18978540380918	-32.06786555106447	7.86315669170687
C	32.24634582483895	-27.62942317162313	7.04012386508335
C	33.48876338756326	-27.99058904612005	6.26596079543091
C	33.72429044050433	-29.42826556153437	6.17024115259679
O	34.53811473351585	-30.01873003926480	5.47976193737689
O	32.87831953610868	-30.18400712209638	7.00705057562569
H	29.77210943159352	-22.62359358900557	4.26256479249149
H	31.05889555243487	-21.89004166543166	5.22708009280633
H	29.95464575782592	-23.04901481745494	5.96795548818824
H	31.14715003100822	-24.28998932627471	1.40404013259858
H	30.07003331160028	-25.51772210850306	2.07122767467473
H	29.79780670929022	-23.81038339898363	2.44039019403994
H	33.74058258357404	-27.24865855054712	-0.22382186957704
H	34.43335621510871	-28.85765767244731	-0.45755202460650
H	32.86185633092876	-28.67493596090425	0.33193504943847
H	36.29562433970871	-29.77485992147626	0.18479757119852
H	37.65973990201193	-29.23592775079748	1.17263711392683
H	36.70009895935257	-30.62801102658586	1.68002513506729
H	33.61835770545802	-22.80750861747891	10.69860891610473
H	32.18058735092735	-23.16592593459310	9.73450544494803
H	33.37766165072596	-22.01693121466449	9.13557649185643
H	36.70951319170116	-24.64258762061894	10.79779660349369
H	35.52765682308898	-25.81584524550866	11.37850838700191
H	39.71382035120811	-29.24809021768594	8.64672367575646
H	39.29844651705218	-27.61354164660962	9.17816775755703
H	38.27714419771777	-28.97626863384118	9.64039232311374
H	38.90847117017191	-30.78096931861858	5.48345920462719
H	39.90169180540614	-29.39599236332393	5.02278133878909

H	40.03605611211586	-30.07640253634987	6.64971346427640
H	35.18362047396888	-24.08599604380482	11.49776718489038
H	34.03062669419177	-31.73258829314415	8.89253245649370
H	34.25685071719598	-33.16278055965140	7.86347920168815
H	35.13916871341530	-31.66278626331355	7.51004916807680
H	33.23854800022579	-31.91059440989193	5.92984958067561
H	32.09657479572788	-32.01553402240130	7.29230056267729
H	32.02310748909350	-26.56725549999913	6.98476042129156
H	31.36565283473137	-28.18784507976978	6.69303794629839
H	32.35811018931479	-27.89408242195303	8.10243357027463
H	32.37942922450125	-26.52702921473056	1.74168162122769
H	36.91421777418244	-26.80026372373259	9.46563754973795
H	37.72420072747304	-29.37363812513208	3.69986664011124
H	32.18972620877424	-23.18726696722477	7.17050601952901
O	35.88706174317617	-25.25415376568380	4.91709929463691
H	35.51831761182547	-24.39089585221722	5.15684067928506

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B3LYP Scan/Hydroxide IPC Model/BSS/180 degrees Constrained Optimization

C	30.54194394228395	-24.66375742528392	2.35770264048071
C	35.70942081840050	-24.76726512370151	10.85397346464503
C	39.42869450786873	-29.73011851804094	5.85454646907885
C	33.84950798123256	-28.32110355934504	0.31201119360169
N	33.15939226153525	-25.51514465209688	4.91013894271110
N	34.63854434307305	-25.54377656457607	7.34213426570191
N	34.94042113016514	-27.50283678384580	3.80835859591715
C	32.94826428223788	-26.58749174907706	2.71899216193919
C	32.80503174418936	-24.01205199729706	6.80935013622424
C	36.46591911882414	-26.66479200385662	8.52579929743317
C	37.04679700100777	-28.67982007159688	4.17839658168677
C	30.49192100801710	-22.87962880494753	5.07799480318987
C	33.30041205877012	-22.92454542746239	9.67615591596583
C	38.98553328720575	-28.44545535274859	8.81554723843281
C	36.66233375674447	-29.65026181329544	1.25948303940623
C	32.54414227807688	-25.68887092779228	3.70365663089013
C	33.79138775621274	-24.51796819214804	7.65465520931427
C	36.94657741876226	-27.46193373103509	7.48978943986153
C	35.95946701018344	-28.30651410500726	3.39775079219665
C	31.43769970891171	-24.75300487846437	3.55830672856119
C	34.04211585903848	-24.04521470765532	9.00846591868128
C	38.15094061312516	-28.28157574791874	7.57959477758845
C	35.74106470276757	-28.74754463481970	2.02529584422378
C	31.41799823441597	-23.99827661132538	4.70149351159674
C	35.05454841727602	-24.82291721977894	9.50522889982286
C	38.33984322411209	-28.81831155736334	6.33624579983837
C	34.55694053140214	-28.19096483692455	1.62818955336232
C	32.50097570928035	-24.49518485820447	5.53747328276058
C	35.42156827307625	-25.74722606799022	8.44181746373810
C	37.23587324788986	-28.34007150011627	5.51255767145773
C	34.08248813259894	-27.39516004811872	2.75610729087303
N	36.41238135061469	-27.53607792341278	6.23907624887729
Fe	34.76023795337879	-26.57365811155567	5.58970533695488
C	32.85492618215505	-31.61643429455217	6.63843168601892
C	33.75562202343090	-32.21447318083246	7.71422817428947
C	32.29375390384353	-27.63944679210564	7.07652881316132
C	33.54211902421314	-27.99503527067727	6.30901975004253
C	33.74928550085606	-29.43277860634987	6.16057504697993
C	34.66087697198874	-30.01423154468269	5.59519917052943
O	32.73353296940872	-30.20217599727489	6.76551833370521
H	29.74620163200825	-22.69245199635128	4.29715005754890
H	31.03359365077942	-21.93762657429746	5.24433138973159
H	29.94423238475312	-23.09733735705052	6.00577518502176
H	31.10136062884060	-24.40053922340858	1.44880530222555
H	30.0369985965716	-25.61823269315354	2.15357872470142
H	29.76321152583451	-23.90477097582981	2.49200272576893
H	33.68731026724726	-27.34352215035234	-0.16322441090889
H	34.42265830544769	-28.93421571050579	-0.39241825137888
H	32.86066243057308	-28.78838402979268	0.42320484434820

H	36.30693558166470	-29.81392775286589	0.23588649557085
H	37.67701192571224	-29.23362885441779	1.19157972233428
H	36.75389834760657	-30.63611636803188	1.73629732496773
H	33.66955186239002	-22.74722724413976	10.69247295688030
H	32.22387787985335	-23.13378407205570	9.75116217634999
H	33.40134558447760	-21.98063518199265	9.12196298005786
H	36.78155647785329	-24.53761860413141	10.77766878564076
H	35.62860653098102	-25.72559174855383	11.38588844722556
H	39.83035300595906	-29.12149242337841	8.64306455658686
H	39.39814293278469	-27.48717239814812	9.16200951072552
H	38.40091200384325	-28.85879156499387	9.64956362056303
H	39.02540511411397	-30.68791583902296	5.49786173333983
H	39.98780861667068	-29.28757529870818	5.01809332243398
H	40.15059224620514	-29.95406347619333	6.64816233824784
H	35.25495817516546	-24.00105784750323	11.49179505106260
H	33.39683762831459	-31.94477028874818	8.71226413659930
H	33.77604664365854	-33.30873122051382	7.63995798758918
H	34.77450003023103	-31.84143346870091	7.59889300106087
H	33.24000186628669	-31.86347179924575	5.64564393996255
H	31.83398450215916	-32.00140715887157	6.73016156922246
H	32.13875911808712	-26.56591831226844	7.13661242228277
H	31.39967959772168	-28.09105312141273	6.62368817954268
H	32.32988921525589	-28.03568694374167	8.10227159393827
H	32.36007624143679	-26.61074528715540	1.80597510032296
H	36.99941811993666	-26.71458142284747	9.47079773846198
H	37.78757812375503	-29.32932412412863	3.72140786594608
H	32.20049117606266	-23.19283769210458	7.18756110894019
O	35.88695387508584	-25.23155050730481	4.92084898235049
H	35.51300180601072	-24.37329161779927	5.17004499843413

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B3LYP Scan/Hydroxide IPC Model/BSS/190 degrees Constrained Optimization

C	30.49975376697614	-24.72055197930636	2.42850951408094
C	35.79953400874749	-24.62459614927786	10.84870302793210
C	39.48494096001176	-29.64282441688108	5.88130570958153
C	33.80076600567891	-28.39150915717089	0.40528878665199
N	33.11733223803762	-25.55421561912183	4.98624703559865
N	34.64085514064151	-25.52151429003534	7.39458639308053
N	34.94648740642273	-27.49142915459210	3.86500212897899
C	32.91568712288362	-26.63056130842518	2.79769907976062
C	32.77572184853906	-24.03017622515857	6.86672621430893
C	36.52660119711155	-26.56904211722240	8.54846975340646
C	37.07557688762299	-28.63780892493842	4.21780556316933
C	30.44804762348470	-22.92173961172258	5.13914011476815
C	33.32331335985730	-22.85964973110124	9.68984526817048
C	39.06310120129007	-28.32396875435416	8.82927819538347
C	36.64429687685671	-29.67013669854886	1.32354757896853
C	32.50513190979326	-25.73409025216852	3.78174033718499
C	33.78788918916874	-24.50180740866438	7.69917394087003
C	37.00538907769815	-27.36926600372303	7.51444651219512
C	35.96744246674179	-28.29577452761614	3.44968538657018
C	31.39200444222021	-24.80413178594878	3.63206407168158
C	34.06389931934914	-23.98859845990201	9.03538862680504
C	38.21653494572774	-28.17640100590845	7.59927031963290
C	35.72954221977292	-28.76133069604180	2.09066607712625
C	31.37190658028281	-24.04455305741935	4.77055122101570
C	35.10371374257027	-24.73243772292442	9.52401412661508
C	38.39682966343513	-28.72837917795358	6.36040894754737
C	34.53063084705865	-28.22479777543936	1.70546845205842
C	32.46217199362125	-24.53193847734255	5.60590655717835
C	35.45935169621841	-25.67742338414760	8.47249427305598
C	37.28049387117505	-28.27284060148879	5.54382445417298
C	34.06455004682433	-27.41750821327095	2.82606179970871
N	36.45917114551440	-27.45931569733786	6.26765460562705
Fe	34.75932931502417	-26.55145989073473	5.64821628795109
C	32.75018850290615	-31.59771905794698	6.26842261036061
C	33.41814196383920	-32.32724267993550	7.42968393603913
C	32.31724204395206	-27.67131091603408	7.14796354638286

C	33.57883762464552	-27.99485357914300	6.38667806174650
C	33.77935289212270	-29.42383049477206	6.16659109688242
O	34.76823676373348	-29.99608861588153	5.73919165922319
O	32.64712744087477	-30.19563955960939	6.50071172094822
H	29.70029809021835	-22.74123188238853	4.35856714496978
H	30.99274405677243	-21.97971546204874	5.29388520709855
H	29.90288338423866	-23.12920268455192	6.07076887454206
H	31.06163265842603	-24.45616847286739	1.52140959272800
H	29.99858120864089	-25.67693729155116	2.22333503904331
H	29.71812393634031	-23.96388250989719	2.55902064908476
H	33.56745090503364	-27.42309975726094	-0.05820138430711
H	34.39327108741944	-28.96425490037536	-0.31698728258929
H	32.84551774818163	-28.91959830526056	0.53649008486456
H	36.28473305643982	-29.83373483414122	0.30139573463619
H	37.66133842166319	-29.26000965640986	1.25124607225996
H	36.73222854589895	-30.65595598054373	1.80128084216739
H	33.70437612433197	-22.65953304330393	10.69754942428216
H	32.24913378354336	-23.07360410144251	9.78256986721525
H	33.41230056225501	-21.92728299898762	9.11460881828622
H	36.85558565181469	-24.34188770044410	10.73376054883658
H	35.78490463140868	-25.57797433103379	11.39519485234337
H	39.91304492442254	-28.99279880001588	8.65413717742630
H	39.46855382675818	-27.35960708540876	9.16705846962319
H	38.48869594626973	-28.73802969339015	9.66981569258520
H	39.08155744564169	-30.60764212931521	5.54439413779264
H	40.03436793855028	-29.21248204537416	5.03191854398382
H	40.21594957681108	-29.85138248802893	6.67070776688721
H	35.32778455843032	-23.87312400609978	11.49150301015191
H	32.88846266464149	-32.12988726208810	8.36664449171654
H	33.42092296694599	-33.41057375430278	7.25747993774477
H	34.45095710318512	-31.99211073684732	7.53642805493061
H	33.30586584906834	-31.77628753629032	5.34398777079469
H	31.71935250085242	-31.94254312047920	6.13706899734637
H	32.27074033543548	-26.62542532075318	7.44098472901518
H	31.43083400018283	-27.88367396970984	6.53107688892232
H	32.20192128047714	-28.29137709713629	8.04727249136583
H	32.31929450140456	-26.66928687997764	1.89053276047464
H	37.07964010765649	-26.59399742155945	9.48316869439697
H	37.81562937962260	-29.28834461178550	3.76126821384202
H	32.16832838312882	-23.21090208681718	7.24037788973610
O	35.79121256490583	-25.13691313143701	4.97795089960216
H	36.54956409754834	-25.51265727446251	4.50619564577925

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B3LYP Scan/Hydroxide IPC Model/BSS/200 degrees Constrained Optimization

C	30.46080832467871	-24.82569341424016	2.49581833529804
C	35.88726112203332	-24.50243706338645	10.83064275992582
C	39.54132761957749	-29.59666293220644	5.92078854503846
C	33.78594389217283	-28.48413462060800	0.48710666199373
N	33.12370908070312	-25.58143867428705	5.03100933938455
N	34.67524409072704	-25.49269192052932	7.42016974445315
N	34.96884673500276	-27.50889328966351	3.91376113642075
C	32.91478545248879	-26.68840577590019	2.85824821960219
C	32.77698070830998	-24.04192270353451	6.89784368571480
C	36.59582752663712	-26.48921650828384	8.56153371797218
C	37.10703367013483	-28.63840656360305	4.26562190546729
C	30.40797081135231	-22.99728833067626	5.18609198947368
C	33.35678257294198	-22.80634053176572	9.68718971137564
C	39.14697074090280	-28.22087316022048	8.84567825580888
C	36.64698224773139	-29.73004399087665	1.39577262723282
C	32.50109905552271	-25.78616567811451	3.83579802919500
C	33.81037321177394	-24.48173390045741	7.72129253570302
C	37.06733381013431	-27.30561337387711	7.53718563824292
C	35.98927460716446	-28.31614040591226	3.50228971255725
C	31.36933298869468	-24.87865225201252	3.68897657183650
C	34.10227235826876	-23.93743719946876	9.04192154711529
C	38.28497905277741	-28.10270309987704	7.62314828938999
C	35.73767206180238	-28.80965867299492	2.15561952509579

C	31.34789212884103	-24.10737451878811	4.81962524896295
C	35.1645000668705	-24.65294838440493	9.52456042395616
C	38.45350889645952	-28.67871227257202	6.39378840952477
C	34.53125354637896	-28.28688923033003	1.77424834964770
C	32.45655145218809	-24.56522234352110	5.64752207485781
C	35.51573760807015	-25.61333002021151	8.48538624835882
C	37.32442977551220	-28.24641858844972	5.58189883885448
C	34.07318887635095	-27.46125892219939	2.88444935261726
N	36.50631550497982	-27.42408957413357	6.29939019362016
Fe	34.78812692324071	-26.54588870695395	5.68678957049772
C	32.6724639899865	-31.52632477200153	5.90289469300126
C	33.05154537615704	-32.38371516019748	7.10593916166482
C	32.37618993823227	-27.69328364123167	7.21699137440064
C	33.63031988629056	-27.99717647171736	6.43500989959626
C	33.80753429698882	-29.41695989154040	6.14608955606756
O	34.82832428840366	-30.01129755589798	5.84526902392718
O	32.60157115781372	-30.14154448852605	6.23347174962201
H	29.64968240950048	-22.83775996051040	4.41111569222932
H	30.93774567733988	-22.04446923254871	5.32586400674822
H	29.87551696713887	-23.20438059393199	6.12512356643621
H	31.00760517823896	-24.56950582761494	1.57728067771826
H	29.96881977871391	-25.79130785582065	2.31276797971250
H	29.67175045165635	-24.07642630496735	2.62428338823024
H	33.53902358556413	-27.52659798451860	0.00839625251183
H	34.37342536568092	-29.06627353296049	-0.23173970599013
H	32.83664128275456	-29.01675282555056	0.64104302642702
H	36.27653834729702	-29.91393242365055	0.38096219204570
H	37.66191043005301	-29.31860571072677	1.30441617651968
H	36.74318344117243	-30.70646650233023	1.89090937126851
H	33.75422986752697	-22.57960034539840	10.68288171637170
H	32.28795734527532	-23.03412569698832	9.80543360719001
H	33.42058632807671	-21.88506107258275	9.09115802293908
H	36.93249346694534	-24.19429430743836	10.68583741408901
H	35.91082813946702	-25.44508487030622	11.39512789081783
H	39.99779765455666	-28.88942130858173	8.67394223346221
H	39.55193935867626	-27.24800504909433	9.15881874910467
H	38.58469887554566	-28.62020440860447	9.70136906543922
H	39.13896966589116	-30.56847669026094	5.60342524340985
H	40.08243386145610	-29.17856215615548	5.05999115368922
H	40.27944916247069	-29.78934567539621	6.70764207242611
H	35.41050731216307	-23.75142266289614	11.47029762673970
H	32.35921303394219	-32.21288232191016	7.93602305928406
H	33.02285873639899	-33.44953114073846	6.84814886512892
H	34.06103782182683	-32.13667509486488	7.43900237270641
H	33.39276369643338	-31.67217266249007	5.09389019533521
H	31.67255229134580	-31.78794624789924	5.54173548511877
H	32.35776330618246	-26.66776954253780	7.57920756822938
H	31.48703370676325	-27.84012198899855	6.58590928121263
H	32.24165884362436	-28.36772234619821	8.07446819451899
H	32.30785827938382	-26.74884970863412	1.95932345710602
H	37.16343186936988	-26.48870035404942	9.48780287175999
H	37.84523251246343	-29.29459663947323	3.81425457504871
H	32.15972087588556	-23.22863594711722	7.26850825181158
O	35.79287873533107	-25.12534663410867	4.98751185500336
H	36.53890609676021	-25.49956130997204	4.4953323672462

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B3LYP Scan/Hydroxide IPC Model/BSS/210 degrees Constrained Optimization

C	30.41889853635011	-24.95409268185281	2.56689959175780
C	35.98075138557558	-24.37021026728371	10.79882664302877
C	39.59202256676317	-29.57180961302160	5.96842784231854
C	33.79537743014190	-28.56095209593235	0.55430671510863
N	33.12812023813549	-25.62548180674184	5.07692595684854
N	34.71661070108323	-25.46462623856595	7.43878883950154
N	34.98771556568466	-27.54574390353489	3.96648243496666
C	32.91936054300804	-26.75556580214122	2.91550675365563
C	32.77102981736186	-24.07290736482348	6.93114450698474
C	36.67473584789323	-26.40303111347433	8.56595065545590

C	37.12911989158939	-28.66798060641001	4.32370247004409
C	30.34937458423201	-23.10983123147284	5.24507029233367
C	33.38359546177473	-22.76257659846146	9.67976145988258
C	39.24240227013496	-28.10892042213728	8.85538243701580
C	36.66219139954170	-29.79127844907291	1.46706392341710
C	32.49733871086691	-25.85423073000451	3.89023277386866
C	33.83405194722232	-24.46827978996878	7.73876360976717
C	37.13251139238695	-27.24712465470722	7.55831016226192
C	36.00785726069539	-28.35677193909187	3.56076712206245
C	31.34192002426294	-24.97619957182633	3.74998048027310
C	34.14122631856356	-23.88953036239490	9.04130504166261
C	38.35620678760301	-28.03449051575960	7.64661182519634
C	35.75221886681433	-28.86654137933945	2.22089894831448
C	31.31291234354013	-24.19872317436238	4.87624502223907
C	35.23144758713704	-24.56859447670370	9.51413052800037
C	38.50526898182463	-28.64835009650960	6.43322480827795
C	34.54358970274750	-28.35009343503321	1.83763341304971
C	32.44284985452636	-24.62176263525234	5.69404001000658
C	35.58169423898927	-25.54364198699611	8.48810766288065
C	37.35990706186202	-28.24605117672335	5.62845779730532
C	34.08671115821632	-27.51447608580742	2.94077148526446
N	36.54929339118272	-27.40733772097435	6.33540256487509
Fe	34.81536174894804	-26.55435102566296	5.72699188398795
C	32.53708637258236	-31.38043024313450	5.56181332158865
C	32.70544629840359	-32.37246391853731	6.70730971689784
C	32.47671888760945	-27.70517126441166	7.36512518372347
C	33.68245065269089	-28.00305804676402	6.50770467870256
C	33.79551698707308	-29.40775893553759	6.12699881315899
O	34.80053358558780	-30.05790528272921	5.90242465407945
O	32.53832134448044	-30.02909982669295	6.01838333905572
H	29.57462304310282	-22.98032698028796	4.48082806778335
H	30.85544794226802	-22.14145882936123	5.36462885696965
H	29.83815366491957	-23.31955759031940	6.19517868720556
H	30.94917272931843	-24.69304717785129	1.64008622495585
H	29.94721070560954	-25.93214383479362	2.39723118102107
H	29.61461769791532	-24.22179285060968	2.69857156955925
H	33.54565960032456	-27.60833400286104	0.06732281908785
H	34.38220928340514	-29.14874063602824	-0.16047011876649
H	32.84740493343650	-29.09375469491432	0.71544027192155
H	36.28848149770162	-29.98697439515440	0.45566752871967
H	37.67502867453385	-29.37664698613597	1.36743550198984
H	36.76442082075111	-30.76215266491375	1.97173087589965
H	33.78649322754614	-22.51766393224456	10.66896149963288
H	32.31983134027134	-23.00609933535614	9.81081298849317
H	33.42700506282605	-21.84740556253695	9.07250103551758
H	37.00496661114852	-24.01113869280372	10.62371474761256
H	36.06664601533216	-25.30507524405045	11.36992045568503
H	40.09216610311944	-28.78010768506114	8.68898184746461
H	39.64980338480829	-27.12489510822762	9.12786457804502
H	38.69894824256528	-28.48129965540025	9.73499181133650
H	39.19083356874845	-30.55135522440299	5.67444330808497
H	40.12372236642054	-29.16905173754814	5.09447076115172
H	40.33824176066479	-29.74565630014028	6.75205593608330
H	35.48401404192060	-23.63811594015935	11.44524101387269
H	31.94385561130127	-32.20899282216563	7.47596565019900
H	32.61243235271852	-33.40366945354889	6.34501316300752
H	33.69020104232934	-32.25427231270068	7.16282475122768
H	33.33229406572033	-31.51654163356491	4.82440630590506
H	31.56849516758109	-31.51645098124012	5.07037312480932
H	32.58213323952982	-26.75846550725782	7.89275955222598
H	31.57583002158388	-27.62796475307169	6.73784991177712
H	32.26437376930089	-28.49357141158529	8.10011754494078
H	32.30593344338033	-26.83349048867734	2.02242499757341
H	37.26056115154272	-26.36957388343167	9.48017038211344
H	37.86441684791046	-29.33206712163104	3.87926614793804
H	32.13886044676088	-23.27071831510006	7.30096152998791
O	35.79626665369148	-25.13790917284718	4.98504192779662
H	36.50440527590274	-25.51765415516295	4.44363753435047

B3LYP Scan/Hydroxide IPC Model/BSS/220 degrees Constrained Optimization

C	30.42650346330386	-24.98765105142920	2.56296455234032
C	35.98382100566841	-24.33380685584902	10.79252226188129
C	39.59410899335860	-29.58640242509325	6.00564594568365
C	33.79154908861632	-28.62224748161458	0.58735785736785
N	33.13474539028316	-25.63724228370949	5.08015599707217
N	34.73483867898493	-25.44095428285766	7.43091760120299
N	34.98928617198684	-27.57675028706203	3.98885873093529
C	32.92705179816047	-26.78466575333292	2.92718756149122
C	32.76575438064604	-24.08126227779287	6.92899994679775
C	36.70165747854256	-26.35972558204532	8.56005138490933
C	37.12710269659391	-28.70248001394308	4.35690072441002
C	30.34257184363367	-23.13517134431329	5.23445012366957
C	33.35907625816264	-22.76780444437364	9.68047983469762
C	39.26765032173802	-28.06669684138422	8.86531011341917
C	36.64912133526845	-29.86253411291495	1.51526388114863
C	32.50612821808352	-25.87448179697338	3.89383175108577
C	33.83612036365346	-24.46033539270481	7.73395642723602
C	37.15637856986405	-27.21667892663802	7.56203452127044
C	36.00442452323100	-28.39923145016698	3.59242318359070
C	31.34759824204802	-25.00157470651866	3.74772641304328
C	34.13533290551042	-23.87932555202561	9.03738115516827
C	38.37705839834115	-28.00789533089966	7.65892121492163
C	35.74460461704988	-28.92451553578071	2.25939080617411
C	31.31211700663052	-24.22070888449812	4.87145344210314
C	35.23782430947534	-24.54056120575841	9.50720840127588
C	38.51617968187243	-28.64623513576688	6.45716265753716
C	34.54004379569376	-28.40319032531516	1.86923949955850
C	32.44306172010422	-24.63501764139897	5.69259919262245
C	35.60213114555944	-25.50881240492092	8.47936788405220
C	37.36844948070859	-28.25357708474284	5.65078205546132
C	34.08891993591573	-27.55123499962625	2.96197863750466
N	36.56672178035227	-27.39615050816991	6.34507592010835
Fe	34.82714994101108	-26.55246893885169	5.73569157287972
C	32.56031765501137	-31.28462453065283	5.39877703749868
C	32.54194857726799	-32.31550804008891	6.52176532268407
C	32.55439920254231	-27.68014445546126	7.47371206697329
C	33.71665908798034	-27.98514659817795	6.55972567508814
C	33.82051623616297	-29.38631693266287	6.16758541025782
O	34.81947438927605	-30.07195791840767	6.05401100555599
O	32.56249360130212	-29.94680379990980	5.89730679580001
H	29.56970596966951	-23.01116671557038	4.46738123618099
H	30.84402029373074	-22.16431060851627	5.35308281721361
H	29.82913899966186	-23.34455160757650	6.18347946984901
H	30.95713487950180	-24.72705762950542	1.63623682882475
H	29.95960918199599	-25.96839087494351	2.39568703887332
H	29.61873150024168	-24.25858449851815	2.69111042454281
H	33.55111737326568	-27.67297331803990	0.08929858330506
H	34.37393021221884	-29.22325209056866	-0.12001713417536
H	32.83851464869234	-29.14439972431909	0.75317185468686
H	36.26993370348496	-30.07256654103731	0.50880234170254
H	37.66226834407755	-29.45152517486045	1.40418777376342
H	36.75235664366424	-30.82602078854931	2.03363184977888
H	33.74595339897044	-22.53305351227938	10.67850997378202
H	32.29604897862364	-23.02283177070338	9.79345733915138
H	33.40228820541756	-21.84365643779104	9.08679701905577
H	36.99789840070334	-23.94590189642289	10.61984913060568
H	36.09512862945038	-25.27142186938362	11.35448249457395
H	40.11700270952861	-28.73962056246515	8.70399230534405
H	39.67535415454989	-27.07927848684172	9.12448048045294
H	38.72756360930128	-28.42895556523731	9.75126262165713
H	39.18580882324431	-30.57182307664801	5.74248169121034
H	40.11786718119507	-29.20953495873543	5.11556148003966
H	40.34809527961593	-29.74234602006981	6.78561581804990
H	35.46862926532579	-23.62139378657820	11.44645751678851
H	31.69115375799377	-32.14669099931491	7.18900008906733

H	32.46331794358783	-33.33090448700924	6.11425866419775
H	33.46138707767927	-32.24883184324800	7.10598237905630
H	33.43485925999381	-31.43574800916424	4.76145596317598
H	31.65635464181616	-31.36127249637887	4.78649814454884
H	32.84721237249897	-26.96347913217183	8.24517112649176
H	31.73982994885196	-27.20266427019714	6.91027466441796
H	32.12825764511473	-28.56486620254510	7.96145513409811
H	32.31438763128981	-26.86792497360486	2.03407966029784
H	37.28984058357145	-26.31524428988957	9.47225951700238
H	37.85684467770353	-29.37893265611695	3.92202647065366
H	32.12402174041834	-23.28653585360662	7.29849326831509
O	35.79985682582397	-25.14846301052247	4.95631074132219
H	36.49259237092841	-25.53751467023590	4.40185799761896

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B3LYP Scan/Hydroxide IPC Model/BSS/230 degrees Constrained Optimization

C	30.38671389754905	-24.95576931617658	2.62185063265357
C	36.03925401812261	-24.29157889173466	10.78561730539938
C	39.54244248700925	-29.62059485184508	6.00514282357365
C	33.66827609266554	-28.67008514870695	0.65865022875103
N	33.10639247667176	-25.62085253044143	5.12289227751472
N	34.72914070222830	-25.42623657134656	7.45659395804427
N	34.93453201718617	-27.58603063762776	4.02200593126644
C	32.86193336896680	-26.78831587279134	2.98452104529810
C	32.77789917909971	-24.03986873025701	6.95759972193749
C	36.70936298104044	-26.34379328610866	8.56242021652145
C	37.06791762441090	-28.72537151183300	4.37390900774034
C	30.36054001243795	-23.06754234956141	5.26953952782457
C	33.41840610136956	-22.70709181851682	9.68969061554305
C	39.25990778505681	-28.07418650020293	8.85513101965806
C	36.52961588653595	-29.92451350411536	1.55496151167833
C	32.46349759109509	-25.86170606565779	3.94523948757150
C	33.84737560426485	-24.43058177936923	7.75920483846771
C	37.15035050104506	-27.20561457998910	7.56232959762036
C	35.93570718877146	-28.42373499679707	3.62120023260903
C	31.31800502418606	-24.97087311609646	3.79846238178604
C	34.17142891646807	-23.83722541333430	9.05133561735339
C	38.36291036665566	-28.00999846158087	7.65388042671220
C	35.64699932867822	-28.96729742078636	2.30143296607721
C	31.30614560606198	-24.17583232589618	4.91227164977131
C	35.27212769241076	-24.50592103838884	9.51400392032259
C	38.48360559834997	-28.65905854886343	6.45629868236180
C	34.44057441957371	-28.43923357714687	1.92431788972542
C	32.43712206849627	-24.60020278177356	5.72862227609180
C	35.61113191438390	-25.49030300838370	8.49271405135218
C	37.33364759823556	-28.25817545848749	5.65696989937681
C	34.01645066214602	-27.56672793457863	3.01103932204072
N	36.55029127300332	-27.38293381126651	6.35036146558726
Fe	34.80188058873246	-26.54426082254442	5.76375718693389
C	32.92606665970416	-31.29971080418843	5.21157605988311
C	32.66606596664113	-32.32766574400686	6.30686038118732
C	32.45095384327524	-27.73196222450960	7.37860717201966
C	33.71099350866930	-27.97078754411906	6.58405714048863
C	33.92258740550468	-29.38301672711048	6.26021731361048
O	34.92331695970191	-30.05398243268242	6.41980272322360
O	32.78424969351214	-29.95951363830802	5.68770192883906
H	29.57864726282957	-22.94385928315325	4.51162545057476
H	30.88004505456471	-22.10341511231397	5.36338298598064
H	29.85755095164968	-23.25099750136809	6.22945846400802
H	30.91478197131402	-24.72387379399679	1.68613073006640
H	29.89534195617316	-25.92800516707258	2.47572282690039
H	29.59721792329077	-24.20587411451987	2.74396008826991
H	33.43665472357495	-27.72653000913991	0.14571017390117
H	34.22889668975655	-29.29500750454489	-0.04551384639201
H	32.70884349836869	-29.17138093377875	0.84957792375129
H	36.12975359001376	-30.14643786355881	0.55908472307283
H	37.54392650175401	-29.52421029950774	1.41853143842220
H	36.63536997238646	-30.88144472227559	2.08511081175847

H	33.83138519378934	-22.45422842274521	10.67274501239052
H	32.35656857853117	-22.95160927424490	9.83367846778733
H	33.45354861906284	-21.79609118362439	9.07554583946908
H	37.05758206034048	-23.92494826532064	10.59261295252266
H	36.14187481556068	-25.22150172929487	11.36197096519198
H	40.10134981259483	-28.75646653475049	8.69160061499284
H	39.67941785651005	-27.09029591858688	9.10900917746473
H	38.72060131638456	-28.42806593375281	9.74488206280129
H	39.11510444512266	-30.60137543551234	5.75524266902307
H	40.06586389480776	-29.26158406082342	5.10746006123623
H	40.29947155786748	-29.78200846014530	6.78101288444755
H	35.54590379998017	-23.55906799316474	11.43420718981113
H	31.67759729657059	-32.17873703553990	6.75216933248248
H	32.71111941082155	-33.34580684319775	5.90133504046745
H	33.41855225127399	-32.23618656164552	7.09180323419048
H	33.92823728333872	-31.43093116907590	4.79726139973361
H	32.19292858175362	-31.39386355977021	4.40495548645904
H	32.37218450689194	-26.70217820136474	7.72372608817668
H	31.56320330798604	-27.95068477737791	6.76714266297768
H	32.38250930649840	-28.39034894517557	8.25963841060505
H	32.23587855560795	-26.87547800358463	2.10104157009931
H	37.30833365500488	-26.29792401060962	9.46757009181565
H	37.78435185096838	-29.41595336470410	3.93899570142328
H	32.15351840730091	-23.22986317036099	7.32370129805537
O	35.76023426675749	-25.14270007325416	4.95756522076407
H	36.49473781607846	-25.53449653301139	4.46185370287971

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B3LYP Scan/Hydroxide IPC Model/BSS/240 degrees Constrained Optimization

C	30.38977572892097	-24.94216416808226	2.62295477923968
C	36.05492745985866	-24.27687324716174	10.77789742104237
C	39.51866223158341	-29.65359410497865	6.01934204715161
C	33.65023271853033	-28.67575661232126	0.66690636387656
N	33.10515845600960	-25.61561970332683	5.12659727376341
N	34.73372431614008	-25.41740808097554	7.45510700004523
N	34.92229854762819	-27.59615191280893	4.02950004594656
C	32.85956549734109	-26.78043179825385	2.98680009315832
C	32.77684016149785	-24.03684048146165	6.96326792883874
C	36.72144270364333	-26.32846938151793	8.55331740150572
C	37.04058501978247	-28.76106750389832	4.39066350937412
C	30.35812712475627	-23.06357680460040	5.27764792263081
C	33.42094128188370	-22.70518701201553	9.69526443847290
C	39.26790409344810	-28.06387704294426	8.84777738240936
C	36.49134346036531	-29.96638419385052	1.57549628639720
C	32.46370732388235	-25.85304759005853	3.94749872691911
C	33.849688575088956	-24.42526151073748	7.76163670538715
C	37.15438568864302	-27.19984572223756	7.55809848271842
C	35.91209469934454	-28.45052798746336	3.63517325278492
C	31.31917806184056	-24.96063166232944	3.80097269483183
C	34.17707727251870	-23.83065044397758	9.05241363789278
C	38.36276817756494	-28.01018894365000	7.65209472429287
C	35.61880134291788	-28.99630453324422	2.31732821652494
C	31.30534218254736	-24.16940459134233	4.91724850543061
C	35.28338672866020	-24.49381361456172	9.50939016491776
C	38.47000165479714	-28.67784409142371	6.46358587506259
C	34.42140751711774	-28.45186164055273	1.93456596845128
C	32.43556219001227	-24.59616356424469	5.73383440904352
C	35.62132959159930	-25.47732541394754	8.48679572863688
C	37.31741922522996	-28.27983714102245	5.66642258094178
C	34.00652348606643	-27.56964935559551	3.01696518370083
N	36.54527561453755	-27.38839158669337	6.35220808720513
Fe	34.79802817840302	-26.54369723612164	5.76738455830902
C	33.05683349409846	-31.27882697707783	5.14490090000619
C	32.59738425982202	-32.28431022489004	6.19433487768607
C	32.47167148891369	-27.73535163706569	7.41985681840952
C	33.71765075761804	-27.95773995577786	6.59996279078504
C	33.94758046271840	-29.37660813823437	6.30680963533731
O	34.90429859265838	-30.06190682330564	6.60850136259872

O	32.88908125618529	-29.92900337354373	5.58828372744742
H	29.57997541299613	-22.93445319352327	4.51679663822261
H	30.87709087574042	-22.10017035751243	5.38108385179173
H	29.85039984246888	-23.25395860858905	6.23377517826723
H	30.91925951218957	-24.70728434436824	1.68876699151911
H	29.89900223580428	-25.91414132811843	2.47307051160266
H	29.59981824525075	-24.19291570468577	2.74608811846802
H	33.43743263837167	-27.73091927560340	0.14812962023995
H	34.20262318339320	-29.31402180497457	-0.03176479587201
H	32.68123922771794	-29.15881614111633	0.85632374900776
H	36.08915030356660	-30.18882588655934	0.58068433996292
H	37.50966907369427	-29.57704176107331	1.43696631057466
H	36.58787405997944	-30.92209446276456	2.10966254449174
H	33.83643540743529	-22.45166916130482	10.67710000345105
H	32.36095301184956	-22.95544057336723	9.84306461812936
H	33.44890378109854	-21.79306769531522	9.08241799067719
H	37.07048486601008	-23.90455568384835	10.58120155636686
H	36.16482761517592	-25.20700751760810	11.35253838295662
H	40.10862646696975	-28.74703600573519	8.68423394068290
H	39.68838645776339	-27.07765061632913	9.09053509689510
H	38.73500709074438	-28.41081091762160	9.74411425345591
H	39.08458107833420	-30.63843118050553	5.79827353531256
H	40.03022866328450	-29.31727506180189	5.10623425403994
H	40.28630837345703	-29.79991760031881	6.78773128389818
H	35.56036090722151	-23.54788451622088	11.42953950705457
H	31.56277289533908	-32.08852231628983	6.49201185083521
H	32.65449615363124	-33.30720361040404	5.80268133287198
H	33.23243498671729	-32.21826643575732	7.07955336949991
H	34.10538136941494	-31.44644901019037	4.88948644791929
H	32.45225693280646	-31.35615947201239	4.23677935692838
H	32.32107170167983	-26.68665646635008	7.67043830429100
H	31.58082106818037	-28.08632633966540	6.87747929920778
H	32.49853869612317	-28.30509415532500	8.36388322097216
H	32.23507482041008	-26.86271267286109	2.10172149249763
H	37.32632425212136	-26.27660954528628	9.45419890187418
H	37.74801182647995	-29.46449613401336	3.96151531812976
H	32.15126581878557	-23.22868997905289	7.33143383095248
O	35.75901251699374	-25.14927558751833	4.94790381554210
H	36.49080398382270	-25.54813661211113	4.45383781010700

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B3LYP Scan/Hydroxide IPC Model/BSS/250 degrees Constrained Optimization

C	30.36011598084594	-24.95624267974118	2.65242505313997
C	36.07950588002990	-24.26508804106521	10.76745896057909
C	39.51531977741039	-29.65698414317575	6.00221600564732
C	33.61393534859035	-28.68684245018579	0.68073049499928
N	33.10048517154030	-25.61174780706333	5.13360592498220
N	34.74353705864169	-25.40704010698355	7.45090593912728
N	34.91206842610175	-27.59380749451428	4.02907199521631
C	32.84499442300852	-26.77779193133945	2.99583258806676
C	32.77100290021489	-24.04235737904969	6.97798214617806
C	36.74690823720455	-26.30472377300141	8.53225668036425
C	37.02087210251305	-28.77658740575535	4.38944420172452
C	30.33035377372368	-23.08653220899757	5.31390595098645
C	33.42151711812398	-22.71669181660437	9.71206533218270
C	39.29944041323655	-28.03301356943772	8.81373699484989
C	36.44802306894353	-29.99615580698357	1.58495325425046
C	32.45214699857117	-25.85167300143408	3.95885396732078
C	33.85278910714829	-24.42429828593719	7.76762548715164
C	37.17260058587120	-27.18080119413907	7.53824941117898
C	35.89107566838486	-28.46125356891565	3.63717546048496
C	31.29910666864322	-24.96843652033509	3.82292059686030
C	34.18441697436150	-23.83105373979714	9.05802165442324
C	38.38107873993587	-27.99137725413742	7.62767526513180
C	35.58656481845744	-29.01462703867135	2.32473081792229
C	31.28619681848041	-24.18094589830109	4.94174570779097
C	35.30131237957137	-24.48417599656942	9.50340486093602
C	38.47343580640395	-28.67391026283305	6.44636665183780

C	34.39263471663799	-28.46176379746702	1.94365544106848
C	32.42648511593719	-24.59981338677531	5.74862318999065
C	35.64022573000442	-25.46141927595299	8.47506338486854
C	37.31316465927699	-28.28230642174374	5.65712674110177
C	33.99056153081597	-27.56883079882166	3.02235687638634
N	36.55069117540788	-27.38034664933400	6.34045476947012
Fe	34.79903246699450	-26.53571138567921	5.76397371010472
C	33.24971509370381	-31.29362407224775	5.13886836665139
C	32.50199382300060	-32.22404234212286	6.08639463310678
C	32.48209236194212	-27.74117938449573	7.42063882487537
C	33.73393814367161	-27.94509513434810	6.60570436475890
C	33.99981156709100	-29.36966132484238	6.36577901290099
O	34.89065778734032	-30.05092080295866	6.83121011561660
O	33.06462624814711	-29.92068690283208	5.49754194147985
H	29.54406173846161	-22.96368370548500	4.56042535706383
H	30.83967238506700	-22.11781686878679	5.41572700167757
H	29.83349809127933	-23.28550043407786	6.27398471802488
H	30.87865995926582	-24.70909564843421	1.71524042011105
H	29.88166663639411	-25.93409732771674	2.50110240026699
H	29.56090485016948	-24.21868092643690	2.78599908446654
H	33.41891416235215	-27.74504539057391	0.14938205254575
H	34.15160040919227	-29.34559985088928	-0.01034735460323
H	32.63585623753924	-29.14734426877115	0.87894157927268
H	36.03443261656096	-30.22887796761512	0.59717429409558
H	37.46606966769904	-29.61183897227777	1.43075505193798
H	36.54750360747101	-30.94591148822452	2.12903876148808
H	33.83589391726726	-22.47012262538854	10.69615976721959
H	32.36333705688458	-22.97540998812390	9.85797986939478
H	33.44310024476962	-21.79824102130453	9.10840949367035
H	37.08668098770203	-23.87275290012973	10.56643369459718
H	36.21039655820910	-25.19855369627045	11.33206239754438
H	40.14097481408201	-28.71418795574213	8.64605969834224
H	39.71861504650980	-27.04345127733540	9.04464748787574
H	38.77764713152238	-28.37553793987460	9.71824155084428
H	39.07921368183956	-30.64671812107376	5.80811783628257
H	40.00979810267120	-29.33777679639877	5.07375474327812
H	40.29677021940547	-29.78742873261343	6.75944011541659
H	35.57729965786194	-23.55130489704609	11.43002860347973
H	31.44231341660245	-31.95624936287250	6.13615513542119
H	32.57736999806961	-33.26523852435834	5.75029720723905
H	32.92273318452150	-32.15709745739714	7.09200363842570
H	34.31679430505807	-31.52437020652009	5.13778090188260
H	32.86498626930887	-31.37803134406744	4.11879871303104
H	32.30380756343244	-26.69278313123034	7.65433685181447
H	31.60013705924799	-28.12130010151075	6.88135121163914
H	32.52243149537818	-28.29603489055115	8.37307251983830
H	32.21486671773062	-26.86292015190105	2.11501610538238
H	37.36014677295213	-26.24661534669112	9.42707540396657
H	37.71998733801897	-29.48909107468582	3.96147675389317
H	32.14097000431220	-23.24107230813584	7.35351326781015
O	35.75420977629886	-25.14312035603652	4.93264630568943
H	36.48715280596033	-25.54311943186071	4.44126392595961

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C	30.35811556323565	-24.96612213032539	2.64884916739934
C	36.09278606607402	-24.23065826989079	10.74917513627627
C	39.49814994624882	-29.67974713771761	6.02816017954455
C	33.62315899274267	-28.68729074968235	0.67979250633830
N	33.09132063291420	-25.62279307819934	5.13736364370368
N	34.73896877891625	-25.40563274315967	7.45099965982545
N	34.90654309104821	-27.60338924801366	4.03711004153372
C	32.84569788261501	-26.78273529159658	2.99527911264407
C	32.76076951677673	-24.04938673659809	6.97837969205895
C	36.74698817132182	-26.29374937977122	8.53207396724853
C	37.00604776305465	-28.80017583475449	4.40937804170776
C	30.31555072083613	-23.10360598806747	5.31506632142763
C	33.42625980440596	-22.69579729395226	9.69470096400613

C	39.29531603313291	-28.02694462463520	8.82370674015029
C	36.44355906759867	-30.01395590060776	1.60115756837726
C	32.44720183439561	-25.86102724262470	3.95997788041275
C	33.84876866289765	-24.42131837991077	7.76412923871832
C	37.16702752840109	-27.18140697078000	7.54598953890095
C	35.88224594436287	-28.47746200087282	3.65107273987043
C	31.29283357058544	-24.97983970344069	3.82273833392274
C	34.18689951829753	-23.81545906763154	9.04706056821135
C	38.37313015733606	-27.99497565175927	7.64028347055396
C	35.58228632652038	-29.02925530553992	2.33696036915639
C	31.27459867669290	-24.19543801010682	4.94362129857029
C	35.30734750881826	-24.46264788927813	9.49188858468023
C	38.45981549536464	-28.69004582263464	6.46578726973191
C	34.39425461622614	-28.46881648566083	1.94858318864142
C	32.41417543869832	-24.61300310524966	5.75233124955400
C	35.64126432564778	-25.44945234266319	8.47080789796123
C	37.29935927667960	-28.30148199064540	5.67522399440264
C	33.99051391705760	-27.57454673013947	3.02557510111917
N	36.54100866532320	-27.39135745877348	6.35204699437725
Fe	34.78976491553615	-26.54461974539265	5.77034229400356
C	33.27888796386107	-31.25740362589488	5.06069235959904
C	32.46233967482461	-32.18757331033398	5.94957898738024
C	32.55883328297661	-27.75148341794777	7.54866692640094
C	33.73485635882493	-27.94858331344057	6.62617447558329
C	33.98065558257785	-29.37693377850665	6.37538718340785
O	34.81500814798125	-30.08784631782036	6.89853171290451
O	33.10205344473054	-29.88576894250596	5.43238477449122
H	29.53073697315617	-22.98148634578431	4.55990862148031
H	30.82248378889650	-22.13387665849447	5.41926182937630
H	29.81692847761963	-23.30483365491585	6.27374969647656
H	30.88037230671994	-24.71811089143320	1.71395285514597
H	29.87988085196224	-25.94362710292665	2.49454259375619
H	29.55876475460364	-24.22831459025182	2.78017979291769
H	33.43488106086826	-27.74297853038721	0.15049374030215
H	34.16331245651533	-29.34530573820924	-0.01007176731780
H	32.64218003746448	-29.14516091816490	0.86958146686921
H	36.03534506535409	-30.24276492035394	0.61024346319071
H	37.46452214607274	-29.63446482459749	1.45435897693034
H	36.53485643938319	-30.96532258341032	2.14388374219811
H	33.84661983701586	-22.43852296780914	10.67350077799697
H	32.36951914904061	-22.95487210180214	9.85014746323573
H	33.44219412830262	-21.78358500556073	9.08150876014198
H	37.09898882541123	-23.84101673956376	10.53831173647096
H	36.22642162394985	-25.15808018271294	11.32306711272088
H	40.13329005363646	-28.71371185613424	8.66108613124356
H	39.71969760015759	-27.03663289483819	9.04151025039760
H	38.77529087002635	-28.35652862832950	9.73400385701477
H	39.05778801120827	-30.66790955521645	5.83574120120594
H	39.99744963181742	-29.36612610399019	5.10032130633238
H	40.27645272166144	-29.81164544360254	6.78836130334290
H	35.59459480149181	-23.50952377546293	11.40681132846765
H	31.40663361150384	-31.90023955497216	5.94446324636459
H	32.53735509085168	-33.22441667345483	5.60032180452488
H	32.82779023078778	-32.14416101569765	6.97767488140456
H	34.33989794864572	-31.50950723043640	5.11218425340678
H	32.94891258990941	-31.31454712264809	4.02003464609565
H	32.33231520965916	-26.69988374473599	7.71769731609174
H	31.65282936901448	-28.23621614732756	7.15053659446528
H	32.74701830233032	-28.21503638228941	8.53188934282562
H	32.21962914491283	-26.86545510887576	2.11134548572028
H	37.36391366007826	-26.22734406548301	9.42377114549424
H	37.70207625627219	-29.51823632298562	3.98566484791761
H	32.12968713240524	-23.24796425428653	7.35187285144874
O	35.74961015012830	-25.15435884816868	4.93867467504836
H	36.45030597862452	-25.56008404115982	4.40668283649695

C	30.36039559689067	-24.88718093737389	2.63197633182756
C	36.08815148989918	-24.24891171920286	10.74445804238081
C	39.42592387237919	-29.737056659733308	6.01988429711493
C	33.56580599268262	-28.66375732616733	0.67052121996297
N	33.07158389826932	-25.59679741136408	5.13024418135796
N	34.71884435517163	-25.40577758516023	7.44632494831831
N	34.86642216215385	-27.59258553451361	4.02505742684437
C	32.81668287828767	-26.74530366774551	2.98334305531443
C	32.75799369352940	-24.02422423568608	6.97472457195037
C	36.72000223522605	-26.31446266371794	8.52363139811570
C	36.94561867936023	-28.82303727295297	4.40026242892579
C	30.33588495984466	-23.03343011667975	5.30488245212502
C	33.43534066399945	-22.68666148194387	9.69554795224568
C	39.24662798443385	-28.07899572481955	8.81441087545683
C	36.37100702657307	-30.02464039109670	1.59082014834600
C	32.42869342667020	-25.82047415280155	3.94955790318766
C	33.83921688884981	-24.41278319438385	7.76176499516040
C	37.12975604849931	-27.20588762717108	7.53701043258334
C	35.82850352496915	-28.48056131464071	3.64031680478847
C	31.28873218491706	-24.92075462114952	3.81045366488451
C	34.18420404883550	-23.81288643080968	9.04551970470643
C	38.32512840083490	-28.03491445199734	7.63097438615723
C	35.52175351147311	-29.02902933803249	2.32602470742933
C	31.27818389468415	-24.13990414030901	4.93383061351758
C	35.29875510955743	-24.47174489573350	9.48803776392977
C	38.40182833045542	-28.73247163895931	6.45713038444854
C	34.34165370253083	-28.45298306312244	1.93751969957041
C	32.40774757607623	-24.57809232316889	5.74552767682782
C	35.62174082200496	-25.46017960277827	8.46506677144740
C	37.24682957580584	-28.32849465332164	5.66650373457531
C	33.95072020010863	-27.55206922986780	3.01418644441668
N	36.50086538180530	-27.40748252295345	6.34265565366209
Fe	34.75832757903951	-26.54051843441206	5.76184374831038
C	33.60789097348720	-31.32560885749066	5.15517076000144
C	32.68825344763270	-32.24211797782715	5.95264532911222
C	32.48661415727155	-27.72780869214471	7.49420767282625
C	33.69693004126621	-27.93782294680815	6.62038956134666
C	33.99959343615106	-29.37247620552301	6.48525617155748
O	34.72314166641421	-30.03787682723985	7.20073403415225
O	33.33404437049931	-29.94385749680626	5.41826193610137
H	29.55579672656142	-22.89641022064304	4.54742409968060
H	30.85836156215387	-22.07246004672666	5.41330465959644
H	29.83066407589319	-23.22874836982339	6.26132897153206
H	30.89033071592963	-24.63758581516658	1.70180823735404
H	29.87199801118224	-25.85795794902899	2.46728890861254
H	29.56854374473844	-24.14160605384436	2.76497783020572
H	33.38875818045521	-27.71830716950256	0.13932196432136
H	34.09597512483477	-29.33032840166561	-0.01886996790364
H	32.57940474982548	-29.10833061668482	0.86378251241183
H	35.95397485927416	-30.25773954650802	0.60458080952509
H	37.39349939289827	-29.65322022563529	1.43373519811743
H	36.46010794734173	-30.97267080046142	2.13971862832931
H	33.86151614239704	-22.43254866598109	10.67265441736400
H	32.37702338072145	-22.93680061291793	9.85492280022314
H	33.45672975472351	-21.77484466531710	9.08194059872243
H	37.09819567362356	-23.86995888484694	10.53239420979518
H	36.21257749111302	-25.17798193283307	11.31771489933643
H	40.07901548717948	-28.77205524292485	8.64971449045705
H	39.67905837710716	-27.09303679023401	9.03592808490514
H	38.72307133816880	-28.40774014016772	9.72291985403901
H	38.97236506320488	-30.72015461605680	5.83155979952368
H	39.92693909020124	-29.43312268843530	5.08976957788600
H	40.20421938472741	-29.87701725247322	6.77857724062772
H	35.59860094380354	-23.52274507027934	11.40303552333827
H	31.63899224625359	-31.99512606498598	5.76505154335921
H	32.84855498166702	-33.29090323708792	5.67529483039938
H	32.88351155249301	-32.13508742255204	7.02135086421247
H	34.65474409860298	-31.53379270523383	5.38533338288536

H	33.44953163717098	-31.4428877604530	4.08008195327746
H	32.25802838274152	-26.67394720606334	7.64516634954281
H	31.59372373050371	-28.20770524544399	7.05935618829702
H	32.62969312407191	-28.18837444951867	8.48581615930190
H	32.19149323134190	-26.81717280680170	2.09778946160007
H	37.33795666521463	-26.25557810508295	9.41512091984720
H	37.63197092242794	-29.54974399276071	3.97535096428267
H	32.13727956746937	-23.21524868506826	7.34930039114981
O	35.72813658239000	-25.15641318371581	4.93259413506624
H	36.44917142405095	-25.56460757927070	4.43047896578974

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B3LYP Scan/Hydroxide IPC Model/BSS/280 degrees Constrained Optimization

C	30.35025229335279	-24.87619891040268	2.63106917590960
C	36.09339630233956	-24.24327394302045	10.73320046000618
C	39.39184217373870	-29.76824516346458	6.02490705526804
C	33.54836423230002	-28.65826944811024	0.66558836088679
N	33.06071427955949	-25.59396301084297	5.12738847437224
N	34.71235002816047	-25.40420580841438	7.44130390809404
N	34.84881549029922	-27.59283651746579	4.02221016681231
C	32.80142516026442	-26.74099672496589	2.98032153614725
C	32.75717081401087	-24.01551113703860	6.96895595806715
C	36.70704565336232	-26.32376807406254	8.52147861517824
C	36.92040917312384	-28.83608678304974	4.40008070291554
C	30.33480419234413	-23.02039555884527	5.30279442584598
C	33.44873014524428	-22.66858342216657	9.68184939343830
C	39.21936560561059	-28.10774672421158	8.81843576316669
C	36.35106473631370	-30.02494867198874	1.58636453895784
C	32.41603000692420	-25.81597396668515	3.94741432764392
C	33.83927647646021	-24.40486962872940	7.75438991759904
C	37.10989348376219	-27.22163780617984	7.53793185238206
C	35.80813957238858	-28.48380543162631	3.63781210565804
C	31.27905065574561	-24.91252278315769	3.80905663071777
C	34.18980209434673	-23.80187440193963	9.03520426351830
C	38.29941054287555	-28.05868349960879	7.63400577839742
C	35.50186113947984	-29.02967690707858	2.32232208679189
C	31.27239464280069	-24.13092152204878	4.93194519646887
C	35.30080147243374	-24.46592658796520	9.47878513236764
C	38.37283665316521	-28.75782338511507	6.46073843641070
C	34.32343758589231	-28.45068899630277	1.93350161132706
C	32.40150593972398	-24.57217184242074	5.74262996190490
C	35.61595654925069	-25.46058298953101	8.45927978341268
C	37.22165338814590	-28.34654067620514	5.66845111803533
C	33.93397073540665	-27.54978259033118	3.01079169030345
N	36.48022734700874	-27.42104227204845	6.34343628227285
Fe	34.74217743012814	-26.54349023598792	5.75841932231569
C	33.73276808755533	-31.32355999758797	5.16390479181464
C	32.73716407311954	-32.24009375539696	5.86357309366629
C	32.52589685499725	-27.71040763383054	7.57657339593287
C	33.67969646321086	-27.93364415084393	6.63196378245810
C	33.98659188441205	-29.36933958407160	6.52256731242862
O	34.62898385935502	-30.03470228706053	7.31333350214398
O	33.43421528170936	-29.94126956008680	5.39695507324845
H	29.55384717493609	-22.88200012541982	4.54650113363832
H	30.86092608021837	-22.06112015104910	5.40851367852237
H	29.83062917654232	-23.21223596485565	6.26047328770540
H	30.88098085437843	-24.63064036074685	1.70028891645733
H	29.85704596302408	-25.84484271336295	2.46808997547457
H	29.56209151222993	-24.12660081545161	2.76328748843713
H	33.37614814401550	-27.71224633288399	0.13379281563134
H	34.07651745791127	-29.32743734769669	-0.02283968513776
H	32.55982437119089	-29.09848884997541	0.85781781780029
H	35.93217487159959	-30.26012434021820	0.60141577446878
H	37.37258468605850	-29.65198205063576	1.42641612152920
H	36.44325502115040	-30.97201265271380	2.13641216998557
H	33.87563773572200	-22.41566310336282	10.65894754458663
H	32.38840520565291	-22.91046494703502	9.84041491885048
H	33.47773657811879	-21.75822436036173	9.06635454226324

H	37.10519471287154	-23.87066569347276	10.51820757900988
H	36.21353464209265	-25.17105807907845	11.30942546218172
H	40.04791657127603	-28.80568442647379	8.65497775269828
H	39.65730629645431	-27.12421790174002	9.03986837068141
H	38.69287427752393	-28.43302082585409	9.72647327841778
H	38.93290787252491	-30.74790092019727	5.83159964229825
H	39.89897647464906	-29.46510500779028	5.09783035240298
H	40.16587954463818	-29.91565520337325	6.78651536408416
H	35.60899284730287	-23.51210824778206	11.39005561677890
H	31.71228655657983	-31.99226635513391	5.57152543602493
H	32.92424116510546	-33.28858832972968	5.60248623988885
H	32.82425088292911	-32.13513500512052	6.94668421172927
H	34.75056131611469	-31.53253169547984	5.49918908326946
H	33.68308891073648	-31.44012713261796	4.07840494477296
H	32.29339243377740	-26.65541963027380	7.71207051799466
H	31.61119866418841	-28.21353963697337	7.21907422059415
H	32.74343754516109	-28.14144061970388	8.56725732110098
H	32.17579416824663	-26.81109773022665	2.09494993081287
H	37.32523877148613	-26.26683419329320	9.41291389755122
H	37.60394359638086	-29.56519108645177	3.97467966087217
H	32.14052440136152	-23.20282746462111	7.34218526641142
O	35.72154533941057	-25.16413173827095	4.93232711054080
H	36.42452482911563	-25.57689011368187	4.40877659738313

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B3LYP Scan/Hydroxide IPC Model/BSS/290 degrees Constrained Optimization

C	30.36974538725362	-24.65352393536272	2.57863222213898
C	36.03155628881614	-24.41909819691863	10.75965319254500
C	39.25581596331224	-29.85884782303221	5.90432658787905
C	33.39482177088524	-28.57382838937056	0.60208990099947
N	33.03513387658207	-25.51476292601494	5.07824518195283
N	34.66136299710149	-25.44024422813468	7.41880906762081
N	34.73229940008583	-27.58185207408942	3.96580126335760
C	32.71878787012160	-26.64599339459674	2.93127508219045
C	32.78505940384113	-23.94946454664376	6.93915450623515
C	36.60585465460213	-26.45965519107148	8.50053784904980
C	36.78877652246610	-28.85913005492231	4.30813455433436
C	30.44412280906943	-22.80439519094001	5.25536887784480
C	33.47301225090319	-22.70939653216456	9.70257716407769
C	39.08357966810788	-28.29645744641960	8.75532611587616
C	36.17396396114397	-30.00572155690093	1.48706483338005
C	32.38163215439018	-25.70095959327253	3.89738047188649
C	33.82625103307717	-24.41263744080796	7.73998346512000
C	36.99431181867043	-27.34050741334296	7.49551751265761
C	35.67521575908196	-28.48015388969621	3.56192922412815
C	31.29259887675062	-24.73954006281887	3.75841706079416
C	34.17906403519858	-23.85619557785859	9.04085193963910
C	38.16940665467637	-28.19819762312204	7.56953728451656
C	35.35218666045189	-29.00037281082451	2.23976214861951
C	31.32420831118268	-23.96056042984005	4.88247352776023
C	35.25274055263652	-24.57766085971344	9.48714396986968
C	38.23978298402258	-28.85937334383438	6.37299522935945
C	34.18306821055783	-28.39509259933713	1.86588780336835
C	32.42513894433221	-24.46358436638642	5.69602083911724
C	35.54451034855758	-25.55984369044668	8.44925950530787
C	37.09702467736597	-28.40921372259995	5.58998305263910
C	33.81833029631435	-27.49974323286049	2.95703504607249
N	36.36522592745929	-27.49388274248621	6.29266806226034
Fe	34.66163401282310	-26.54763497216261	5.71406600255032
C	34.54394032382530	-31.37665190029456	5.84948102730916
C	33.44912943395078	-32.39441235316594	6.14245579029102
C	32.18055655778310	-27.65050241415827	7.20078499801096
C	33.53217194686312	-27.89591276364767	6.57990656468468
C	33.98294460512204	-29.27157673078064	6.83985553765952
O	34.32738907388523	-29.71437951264823	7.92205352037813
H	34.00269227589713	-30.05776262827103	5.71106156940663
O	29.67110771577548	-22.62562824685720	4.49956320792326
H	31.01802859295137	-21.87313078653122	5.36260910377123

H	29.93115376304165	-22.97243042836299	6.21279061918445
H	30.911113122075130	-24.41184673362460	1.65291708526802
H	29.84504593388669	-25.60261978126746	2.39998742548074
H	29.60619264452419	-23.88049461923385	2.72019191640677
H	33.24013726403589	-27.61988092570455	0.07909546152628
H	33.90255254912318	-29.24918439203534	-0.09550925208915
H	32.39788858791138	-28.99336882825411	0.79789758901039
H	35.74718673220728	-30.21526022069356	0.49974043557766
H	37.20465781640073	-29.65743803536031	1.33033045043723
H	36.24197769848182	-30.96371755257550	2.02193416795300
H	33.90396581413631	-22.48535781436799	10.68489946645039
H	32.40472495416667	-22.91930182643338	9.85348373436787
H	33.53406086225977	-21.79123400176650	9.10123394343090
H	37.06759248718825	-24.10444803951803	10.56873060778465
H	36.08534975328005	-25.36004328465255	11.32431537544731
H	39.90580187979602	-28.99733890581382	8.57331569151914
H	39.53075171647893	-27.32530099783237	9.01010630205224
H	38.54855824401562	-28.64470727006756	9.64961476349125
H	38.79427505118791	-30.82633017028643	5.66198818496366
H	39.77474691604784	-29.51844715130382	4.99691795439881
H	40.02041069167171	-30.04493790007433	6.66686076371971
H	35.57850300100768	-23.66905796460918	11.41757487107077
H	32.66097377189475	-32.34076053413890	5.38568755298134
H	33.85564577594538	-33.41291336132709	6.14408324935092
H	33.00339245257916	-32.20068338790897	7.12080926834953
H	35.29421833653136	-31.37634562922062	6.64197774098780
H	35.03122681015928	-31.58595803109115	4.89366261977755
H	31.90666461153672	-26.59684857137731	7.20871051890089
H	31.39232044097941	-28.18976855325620	6.64763631346552
H	32.14592918807982	-28.02657386350882	8.23469529666299
H	32.09075053534438	-26.68528121778469	2.04561072486282
H	37.21514186839510	-26.44597757845809	9.39970218748678
H	37.46513021773162	-29.58161957812422	3.86020626366658
H	32.20363293253246	-23.11392571503503	7.31820691814937
O	35.69545016207731	-25.20118389451500	4.90461440230253
H	36.50358185971678	-25.61351358906722	4.56459886301962

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B3LYP Scan/Hydroxide IPC Model/BSS/300 degrees Constrained Optimization

C	30.35334033336321	-24.66717172519955	2.58960694712227
C	36.03498169990622	-24.42579849271923	10.75681338578241
C	39.24257009840827	-29.86900821749158	5.90595860100578
C	33.38184763537378	-28.58145064603400	0.60662256993204
N	33.02387907509115	-25.52448317010400	5.08458906037896
N	34.65151908875945	-25.45236599092865	7.42324503340641
N	34.71576783553483	-27.59416582692071	3.97331030444156
C	32.69419189615118	-26.66830038992974	2.94618360566322
C	32.80183632408600	-23.93353559039005	6.92691862577478
C	36.57612246023612	-26.49537412865999	8.51828176728474
C	36.78522844983910	-28.85330318544156	4.30416668578841
C	30.46255694317970	-22.78547956690056	5.24270867174648
C	33.51444632035657	-22.67291000591422	9.67456810179534
C	39.04551190169016	-28.34392611357123	8.77595254882380
C	36.18212778592677	-29.98188292104792	1.47440067248239
C	32.36324121618939	-25.71740518049266	3.90877629711336
C	33.83663752560393	-24.40457977608085	7.73181040905585
C	36.96281641481821	-27.37749467359584	7.51338641328010
C	35.66897809617486	-28.47755961072228	3.56075565839288
C	31.28210742402337	-24.74777518759845	3.76507709802654
C	34.19861248257324	-23.84100928902912	9.02708390458729
C	38.13821545064116	-28.23500327438974	7.58578332133762
C	35.34984745903574	-28.99172464688598	2.23553396022484
C	31.32867934595339	-23.95501945525051	4.87895645905797
C	35.25529795746498	-24.58055999848846	9.48431248959568
C	38.21932822918395	-28.87976467813723	6.38072156993911
C	34.17105897668815	-28.40050929777530	1.86951227109533
C	32.42872656727145	-24.45950111560088	5.69265722386343
C	35.52949121914997	-25.57902768684343	8.45731172076266

C	37.08050444814348	-28.42296416276059	5.59565588849658
C	33.79875779988389	-27.51605216806841	2.96722293344623
N	36.33995677819630	-27.52117162158047	6.30600443513553
Fe	34.64392264547209	-26.56483321757859	5.72318708695887
C	34.64083541251402	-31.34185025734242	5.88126050277405
C	33.54634311791349	-32.38576343066309	6.06010879344989
C	32.15891212290556	-27.60175657111107	7.23779931313350
C	33.48986467625391	-27.90302608159456	6.59500215738275
C	33.89339241899977	-29.29142771030874	6.85307577017038
O	34.07441680256542	-29.78382052894906	7.95646029172280
O	34.09586824675142	-30.02910854829628	5.71249888745657
H	29.69376367377968	-22.60132942573112	4.48392040602692
H	31.04819404006178	-21.86115036260364	5.34578135955111
H	29.94505775128361	-22.94125383979476	6.19978772106442
H	30.89321386107597	-24.45360006712309	1.65620041962872
H	29.80992039086609	-25.60959299944821	2.43256938919377
H	29.60508642359023	-23.87758531769791	2.72085172379134
H	33.20693220605927	-27.62524077787160	0.09441044135507
H	33.90017075761283	-29.23946808938253	-0.09971436907629
H	32.39401003743717	-29.02251473108620	0.80126160030528
H	35.76367491922846	-30.17929115973794	0.48102423411321
H	37.21205184379011	-29.62615641665118	1.33030937619533
H	36.25108127175571	-30.94738464350102	1.99563246935101
H	33.96496492395015	-22.43062925819400	10.64366764281930
H	32.44711449589212	-22.86925025497550	9.84919278702434
H	33.57295485374338	-21.76980609155380	9.05084161640522
H	37.08684601150790	-24.17276929554408	10.56198216036123
H	36.03693305148868	-25.35092183407287	11.34983412436738
H	39.86348555760418	-29.05024358703522	8.59590934102731
H	39.49876275518232	-27.37689294646719	9.03589681664256
H	38.50351432266113	-28.69071432261238	9.66655755619131
H	38.78604768429651	-30.83337361186941	5.64275641051107
H	39.76983495835634	-29.51209917383000	5.00974347564389
H	39.99996984052240	-30.06566968900355	6.67300670716275
H	35.61949599844794	-23.63336874361155	11.38932905979827
H	32.82995465259423	-32.33899928226253	5.23441725060974
H	33.97421221930983	-33.39519721470273	6.08701788405524
H	33.01024699392970	-32.21338192998508	6.99566459547849
H	35.31894436567883	-31.34327144255019	6.73676408955546
H	35.21588778911966	-31.52544951032149	4.97012541281848
H	31.98278292589688	-26.53463851365464	7.36414188980142
H	31.33381174707207	-27.99171772575063	6.61743326017601
H	32.07150107374036	-28.09048253925203	8.21846438893218
H	32.06251033759182	-26.71075032791432	2.06326862964799
H	37.18150166840121	-26.48667855868477	9.42012944698209
H	37.47066142924957	-29.56245809222909	3.84878572239484
H	32.23397760713816	-23.08487016745642	7.29718026471456
O	35.68832108391355	-25.22698944573819	4.91610251443834
H	36.47577294689528	-25.64852801270111	4.54077008505221

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B3LYP Scan/Hydroxide IPC Model/BSS/310 degrees Constrained Optimization

C	30.33744009327942	-24.68651351498019	2.59675491120262
C	36.02847486921655	-24.44114592237666	10.75657728806806
C	39.24724796963373	-29.86256484799121	5.89365787599657
C	33.37250149277055	-28.59187738956263	0.60665882896540
N	33.01677683874189	-25.53398806223036	5.08526777598813
N	34.65051366826387	-25.45748080478732	7.41773775031553
N	34.70713523329727	-27.60450437707998	3.97306043325996
C	32.67810414536347	-26.68770784445460	2.95315681477597
C	32.81027277469632	-23.92861270143558	6.91621010709139
C	36.56343654907521	-26.51408510972915	8.52020418942683
C	36.78892147584278	-28.84615706885217	4.29308487687416
C	30.46503564222235	-22.78636973176236	5.23621391049557
C	33.53134365073929	-22.66311300359572	9.65968534045937
C	39.03351695943302	-28.36293324925832	8.77595286224658
C	36.18808506930326	-29.96948139394610	1.46176686068982
C	32.35056109493116	-25.73327321276652	3.91357527533474

C	33.84389421381494	-24.40164350980442	7.72157805287952
C	36.95170673215770	-27.39381352580766	7.51361787648127
C	35.66754505461814	-28.47710747990128	3.55430889960010
C	31.27122961375751	-24.76181604616708	3.76858847276784
C	34.20753397736040	-23.83826139254396	9.01652919540707
C	38.12956726012179	-28.24828733861801	7.58372637712741
C	35.34897013595741	-28.98934930365692	2.22827184149437
C	31.32584594756721	-23.96101709129510	4.87640734683248
C	35.25468007756113	-24.58779365199691	9.47954546173479
C	38.21777539429341	-28.88211961394409	6.37324447984719
C	34.16307694998198	-28.40860170693974	1.86836488289038
C	32.42811868009471	-24.46293275705053	5.68840844175011
C	35.52353744044362	-25.59030569032095	8.45526589885952
C	37.07914074147503	-28.42433496880691	5.58842928751408
C	33.78662833099398	-27.53064521176683	2.97003548052929
N	36.33208513426668	-27.53263946985688	6.30406220801537
Fe	34.63805127561518	-26.57356428213457	5.72122864920246
C	34.70402950127287	-31.32552816440370	5.95134413034123
C	33.58490489660868	-32.35869483707149	6.00540868701044
C	32.16657917897561	-27.55336276386959	7.28333053928368
C	33.47069573901416	-27.90644362041548	6.61073293056990
C	33.83999586028897	-29.30022500076214	6.87553782578512
O	33.86979324896094	-29.83222769810803	7.97789340612231
O	34.19704750424720	-30.00382600979061	5.75156343369599
H	29.69832109725944	-22.59999811173878	4.47588695121032
H	31.05524417949882	-21.86489642819373	5.33821789939524
H	29.94529907430582	-22.93759066159832	6.19281886947325
H	30.87567231598356	-24.49425316441177	1.65785744520260
H	29.78063334371762	-25.62378658971981	2.45639586830654
H	29.60053285792885	-23.88505477729333	2.71969732067382
H	33.18767735858089	-27.63523404490487	0.09878329033923
H	33.89550627767647	-29.24208729482741	-0.10344856797066
H	32.38923131735184	-29.04295277880398	0.80140996382303
H	35.76917633183604	-30.16731648155914	0.46867702314960
H	37.21449872569880	-29.60420201604245	1.31657519786982
H	36.26647757503449	-30.93578167148675	1.98008982638464
H	33.99169219552422	-22.41245820973130	10.62199414305267
H	32.46547306870586	-22.85611653575208	9.84674185095569
H	33.58512401459095	-21.76631242836786	9.02668454298699
H	37.09003539995098	-24.22843730979894	10.56714878684626
H	35.99290698472782	-25.35668397441057	11.36349876733123
H	39.85590980886771	-29.06316314230665	8.59240483972428
H	39.48051912347064	-27.39577874923073	9.04593682630444
H	38.49069096653742	-28.72038277390703	9.66189852555824
H	38.79639913212970	-30.82726904377583	5.62211270472803
H	39.77468975579949	-29.49609541381833	5.00144464142818
H	40.00386323359322	-30.06108157484063	6.66100185829634
H	35.63573174723701	-23.62516062066107	11.37346657032763
H	32.95591838406948	-32.29253053058256	5.11258945887419
H	33.99654490540597	-33.37367805951540	6.06215137355180
H	32.96090189472272	-32.18923908613284	6.88477282709268
H	35.29585777024473	-31.35328442082820	6.86872711526716
H	35.36152782104968	-31.50317065886045	5.09653602749851
H	32.10242823267183	-26.49830281994010	7.54893980498654
H	31.32324555389479	-27.75660469056738	6.60229753888925
H	32.00178175212885	-28.15437220210085	8.18659668209767
H	32.04277198577485	-26.73369104949191	2.07303025106601
H	37.16536714442569	-26.50982356412446	9.42438776446666
H	37.48059157190486	-29.54574740350436	3.83229479269594
H	32.24812224813294	-23.07464225895394	7.28287528079834
O	35.68322865936279	-25.24183052161997	4.90959574792578
H	36.45351492694253	-25.66822310975334	4.50522062445935

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B3LYP Scan/Hydroxide IPC Model/BSS/320 degrees Constrained Optimization

C	30.33007897742390	-24.67943722810468	2.60827832279331
C	36.02792642993432	-24.46850894320764	10.76316820474578
C	39.26176242522459	-29.84035475802414	5.86043844523533

C	33.33078664444501	-28.61769939011639	0.62307023585896
N	33.01949248147194	-25.53118710224804	5.08444451949731
N	34.64940899174807	-25.47148480161579	7.42038483176793
N	34.68849475827817	-27.61863138886004	3.97636549838628
C	32.65767948949994	-26.69794959794974	2.96349289653604
C	32.82400832593591	-23.92527153151070	6.91568371055058
C	36.55741936009171	-26.53742328038746	8.52168071815616
C	36.78089495104226	-28.84549993846241	4.28089362317021
C	30.48488795201776	-22.76822592565726	5.23858022816303
C	33.54780921351979	-22.66956534882019	9.66199567055078
C	39.04319134865692	-28.36701850932029	8.75531789496853
C	36.15737395787960	-29.98450528123545	1.45946735079170
C	32.34471421570190	-25.73265688491140	3.91819960950981
C	33.85056529107638	-24.40898997643844	7.72338372139579
C	36.94627184499077	-27.40982250256292	7.50881698690790
C	35.64967674274106	-28.48747564880501	3.55184368411238
C	31.27056611848700	-24.75505208287159	3.77472831262313
C	34.21576951170533	-23.84981132867924	9.01948465351277
C	38.13204874480824	-28.25435405503331	7.56828027157467
C	35.32221289771427	-29.00390137066683	2.22961607098767
C	31.33650654419707	-23.94961003076329	4.87869743475849
C	35.25583525911317	-24.60817198648638	9.48431618346817
C	38.22228205456885	-28.87628889759046	6.35182447887926
C	34.13121864171858	-28.42832183731998	1.87767397506181
C	32.43917669917491	-24.45570443347524	5.68735732030254
C	35.51979041653719	-25.61100802060723	8.45942066922192
C	37.07505797453919	-28.42464394082362	5.57557734264831
C	33.76160800852565	-27.54720459148548	2.97896898253873
N	36.32283194216726	-27.54548481535504	6.30104488936752
Fe	34.63168796994753	-26.58371308400711	5.72163360327239
C	34.80562475674787	-31.30826023394610	6.14227189739277
C	33.70233818247001	-32.33910464804826	5.93232538948386
C	32.10503614482253	-27.50852591590220	7.20058239509317
C	33.43127383626571	-27.91119067964684	6.60176573152286
C	33.75017920965175	-29.30740977988157	6.90249465050655
O	33.54914920317520	-29.87305107015108	7.97261614323653
O	34.35319790990935	-29.98125620753705	5.86895695234372
H	29.71739529253485	-22.57795378351466	4.48005760174374
H	31.08191798721978	-21.85080135988224	5.33708088996728
H	29.96679740701794	-22.91400826412463	6.19689105990743
H	30.86359728635752	-24.49561300523802	1.66503838677531
H	29.76615267775881	-25.61365087189669	2.47640038834940
H	29.59924902030624	-23.87254543754739	2.73183650740446
H	33.14593375633944	-27.66414360220437	0.10936957911566
H	33.84595421969864	-29.27539442652790	-0.08580759899009
H	32.34722187865113	-29.06330176313801	0.82845706209663
H	35.73169669167567	-30.18517087346616	0.46981947301256
H	37.18205507001795	-29.61777904122593	1.30609738366039
H	36.24079087746924	-30.94929018448057	1.97966627818081
H	34.01072124523068	-22.42082600945634	10.62355628346321
H	32.48090087345372	-22.85534954255574	9.85028417188744
H	33.60696085970894	-21.77392939058536	9.02787339715402
H	37.09299891431021	-24.27216143723480	10.57604360294947
H	35.97700122810366	-25.38119652094643	11.37330259497439
H	39.86736465688679	-29.06370158049269	8.56641102512308
H	39.48778401868728	-27.39836595648477	9.02397655980656
H	38.50724222982443	-28.72749275457552	9.64425711688981
H	38.82358343070859	-30.81082408884878	5.58848457318343
H	39.77691231510025	-29.46263340731863	4.96582713928794
H	40.02701000572683	-30.03065942899181	6.62127189222879
H	35.64556721490241	-23.64456965488139	11.37599146068666
H	33.28112339800909	-32.25186135190040	4.92639877810710
H	34.09432251409230	-33.35607088731634	6.05528227857902
H	32.90226977717900	-32.18766574639210	6.65919160760461
H	35.18848457699450	-31.36036811514647	7.16379707162117
H	35.63004493002652	-31.46883590252110	5.44239910939682
H	32.14555204453114	-26.52224137648268	7.66863614628409
H	31.34646504876359	-27.43250708886925	6.40679439586210

H	31.74575520130182	-28.23013489682016	7.94275490461325
H	32.01624347467025	-26.74598529708395	2.08791669567914
H	37.16084832535608	-26.53632826492457	9.42486483848399
H	37.47624310048344	-29.53711849789471	3.81353135990638
H	32.26806014968474	-23.06734396740385	7.28247470546460
O	35.68453289380835	-25.26155878541096	4.90704083259192
H	36.46631913248022	-25.68842393069724	4.52588628805270

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B3LYP Scan/Hydroxide IPC Model/BSS/330 degrees Constrained Optimization

C	30.32804291764089	-24.67598692801125	2.60729425674281
C	36.01863090897309	-24.49228797410609	10.76728463222837
C	39.27184621201872	-29.82361760738272	5.83506744269859
C	33.31109740553426	-28.62960129896303	0.62475515723259
N	33.01766682998606	-25.53552805857958	5.08062349189229
N	34.64764554843360	-25.48142029253795	7.41738551264925
N	34.67036253091209	-27.63598107810303	3.97910191324414
C	32.64226118658625	-26.70956278978044	2.96624522793781
C	32.83225754802285	-23.92471288741940	6.90884913809427
C	36.55052973733893	-26.55455570530300	8.52036162188029
C	36.77295488756361	-28.84835329791778	4.27240507567776
C	30.50067332743574	-22.75626416488565	5.23039388606556
C	33.55296966473818	-22.67720460757701	9.65937233208897
C	39.04847015567064	-28.36985276876952	8.73932459299898
C	36.14394947440486	-29.98885607471515	1.45263986502780
C	32.33843665932167	-25.73755475397973	3.91702512385489
C	33.85399058343555	-24.41445664027934	7.71885718424378
C	36.94157921307162	-27.42076613966564	7.50287210095826
C	35.63440040937260	-28.49985723755012	3.55040946831074
C	31.27033154788663	-24.75353185268222	3.77215297515314
C	34.21774701747378	-23.85922246878752	9.01686350647727
C	38.13295921664267	-28.25823855914747	7.5555620084380
C	35.30546789503497	-29.01523472475951	2.22813135270702
C	31.34406511630424	-23.94428495193658	4.87286876274917
C	35.25167913531388	-24.62433412799744	9.48455707331981
C	38.22503827540614	-28.87186982563824	6.33515070534047
C	34.11179429047230	-28.44270638821204	1.87961478230181
C	32.44497945731430	-24.45463302407086	5.68120280460981
C	35.51440969607529	-25.62640070969599	8.45886117344614
C	37.07188289177898	-28.42471732004712	5.56481856493538
C	33.74252762752028	-27.56365047729791	2.98245824501479
N	36.31670636629185	-27.55336657999856	6.29602079322708
Fe	34.62328331247331	-26.59469969464233	5.71998896119311
C	34.84726428127802	-31.29966900918503	6.28276590518059
C	33.77732012164417	-32.30174550733193	5.86281479154701
C	32.09103707658334	-27.47875839826170	7.20722268659908
C	33.40884017275310	-27.91502749397635	6.61373369423429
C	33.69844496817984	-29.31259569829869	6.93659835588070
O	33.33680943836334	-29.91302766570466	7.94605993697430
O	34.45928229104406	-29.95777001422954	5.99207999200823
H	29.73426852666312	-22.56247244621044	4.47169366598469
H	31.10402604432742	-21.84277465635155	5.32661111174971
H	29.98193805893515	-22.89643440658141	6.18918116178601
H	30.86065078640049	-24.49625305888227	1.66274525480210
H	29.75982622272796	-25.60795627378833	2.47826821092988
H	29.60098586316478	-23.86568194358622	2.73067421178875
H	33.13141584650751	-27.67566898216961	0.10984229352662
H	33.82346786778473	-29.29054900527356	-0.08309399748944
H	32.32518617445598	-29.06993524610672	0.82997677683888
H	35.71309928143655	-30.19392297098860	0.46614624610476
H	37.16402212454398	-29.61259259586653	1.29160558232622
H	36.24009152765332	-30.95224429428185	1.97295568683556
H	34.01435658413707	-22.43182869862153	10.62251643584570
H	32.48485225046893	-22.85902965726190	9.84454272041697
H	33.61741886808844	-21.78089563874571	9.02674404696686
H	37.08642897335549	-24.30597813334756	10.58567140898250
H	35.95589738910797	-25.40472094819573	11.37673538173888
H	39.87403658572968	-29.06386034242126	8.54664777488047

H	39.49120451385312	-27.40028133991198	9.00781462019950
H	38.51683569097267	-28.73300417429563	9.62977227084469
H	38.84198464704816	-30.79567840835392	5.55560049625487
H	39.78292999403468	-29.43437619446230	4.94303797125781
H	40.03945452031320	-30.01349535679870	6.59361285513069
H	35.64098251039373	-23.66503038609901	11.37854150213156
H	33.51608398510385	-32.16286850686663	4.80961841146904
H	32.13392619214513	-33.33016130045348	5.99762640601697
H	32.87783426983880	-32.16550885737803	6.46578157120312
H	35.06391417464879	-31.39605905255137	7.34903840890245
H	35.76869473061670	-31.45200065206612	5.71432118265695
H	32.17674697829069	-26.52409330222571	7.73303380559537
H	31.35964586451405	-27.30914230978599	6.40390675554161
H	31.67552610444545	-28.21967560221326	7.89764693763927
H	31.99888502274750	-26.75726621896893	2.09208155234814
H	37.15302309136135	-26.55687150158382	9.42416695473581
H	37.47091032740563	-29.53416447281715	3.80045610685109
H	32.28091337709161	-23.06319623430992	7.27410655777026
O	35.68094616123209	-25.27900569124737	4.90277939182492
H	36.47286262515712	-25.7049988450059	4.54210232204048

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B3LYP Scan/Hydroxide IPC Model/BSS/340 degrees Constrained Optimization

C	30.28816117347040	-24.76452602108053	2.66420416451853
C	36.06033324738104	-24.42340362537104	10.76065683143052
C	39.29868744555173	-29.80409542479944	5.88175685190023
C	33.28883742059265	-28.71990869861035	0.70450398309871
N	33.02421090937967	-25.55234726750579	5.10971312113344
N	34.66661679289030	-25.46456671753813	7.43590780104000
N	34.67943573837236	-27.65714403455182	4.02437047256683
C	32.62676810521882	-26.77133105787423	3.02506053801089
C	32.85604664803281	-23.90811162500818	6.90927377957014
C	36.56736791593591	-26.53011473905691	8.54953870068882
C	36.79463781963652	-28.84741618374386	4.31552866746936
C	30.49521913285418	-22.78398021821601	5.23949227630385
C	33.60195141788294	-22.61173976554000	9.63132247878350
C	39.06839419100763	-28.34059255706536	8.77999160921144
C	36.15560789568908	-30.02301039788649	1.51170757811232
C	32.32847270272164	-25.78338081405985	3.96133657688014
C	33.88158807463886	-24.38645229226002	7.72118836063692
C	36.95606614321694	-27.40686379824382	7.54006885321232
C	35.64930751995022	-28.51455934398156	3.59644523478853
C	31.25194333303076	-24.80917568323380	3.81314684179343
C	34.25473592828077	-23.81048567777010	9.00760223180853
C	38.15124939910086	-28.23905747266941	7.59652485106140
C	35.31131396347011	-29.05259733356480	2.28544706825840
C	31.33960667175800	-23.97489090335789	4.89418102180609
C	35.28444195669801	-24.57518079863936	9.48540068900309
C	38.24663341888932	-28.85632686955135	6.37840654115220
C	34.10388925400421	-28.50319476041791	1.94535461479602
C	32.45537052621663	-24.46224361949099	5.69637893898888
C	35.53599956245424	-25.59728374489191	8.47664449345558
C	37.09085988723794	-28.41805642269495	5.60658502817716
C	33.73753520499834	-27.61214614108046	3.03950001666425
N	36.33100306083100	-27.54889363470993	6.33507085692873
Fe	34.63539376482395	-26.59980323910787	5.75403268143257
C	34.76363638277213	-31.31446685856790	6.18236858145861
C	33.75549458291562	-32.18359130038588	5.43833731354794
C	32.11583071101339	-27.44421406306277	7.28204534735249
C	33.40583306763242	-27.91216510201531	6.65345516872557
C	33.60142703646275	-29.34719250975705	6.87457650011001
O	33.06145383210268	-30.03499148242965	7.73994164734277
O	34.49400768890359	-29.92605276830610	6.00533871529574
H	29.71620127998079	-22.61025475834202	4.48884226224559
H	31.09498605456681	-21.86559075695101	5.30709983831235
H	29.99205750576893	-22.90660137836424	6.20889607414313
H	30.80195598108035	-24.60381970637031	1.70592920382395
H	29.72394882658169	-25.70282485513101	2.56773353642496

H	29.55792339453936	-23.95625475067611	2.78198330837814
H	33.10866310920071	-27.77983144150930	0.16462796102167
H	33.78985562979643	-29.40377695375665	0.01046874531012
H	32.30299639478483	-29.14850799679930	0.93285814285231
H	35.70824756808868	-30.25879708815773	0.53953165767964
H	37.16268731173483	-29.62646125267910	1.32029791383590
H	36.28618547765431	-30.97235408081677	2.04976301566023
H	34.07013902163204	-22.35223254589459	10.58746857963178
H	32.53347435153194	-22.78202274158216	9.82518476086807
H	33.66985157311758	-21.72778304892703	8.98196745121992
H	37.12598641900725	-24.23517402246965	10.56840734528205
H	36.00634143711761	-25.32783792161471	11.38275826842994
H	39.89345501699447	-29.03651619800861	8.59210645654308
H	39.51198966180513	-27.36892072726717	9.03946859762115
H	38.53829072783015	-28.69579355314706	9.67458566842369
H	38.87337678636018	-30.77768819440051	5.60072835726839
H	39.81145812177418	-29.41294178674045	4.99150548062296
H	40.06452726593726	-29.99126287986601	6.64279900889944
H	35.68404021158151	-23.58965814558933	11.36387775564683
H	33.71059350002177	-31.89697862210345	4.38375516745107
H	34.03580124836917	-33.24238186798159	5.49773911382477
H	32.76169194813959	-32.06439636441919	5.87403455181894
H	34.76445341413672	-31.55625297232851	7.24777632405694
H	35.77058293753898	-31.45691965463787	5.78029350168824
H	32.23585941631566	-26.48863857313474	7.79718955311269
H	31.36349598613422	-27.26724599511396	6.49912763216198
H	31.70308768961249	-28.17620961233783	7.98261131434293
H	31.97043884001794	-26.84256734891714	2.16221630636933
H	37.17210726581768	-26.52250548155961	9.45187959542260
H	37.49697643578187	-29.52993567069391	3.84529267183441
H	32.30920909067715	-23.03879993663166	7.26265751694534
O	35.68984941502087	-25.29257630853032	4.91995994119853
H	36.45675330892684	-25.72771338144964	4.51846973311091

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B3LYP Scan/Hydroxide IPC Model/BSS/350 degrees Constrained Optimization

C	30.28240303134231	-24.78782860434619	2.67715012333787
C	36.07866689170915	-24.39359272239405	10.75464806870758
C	39.30904806642172	-29.79190686488709	5.89522856720417
C	33.28395666754902	-28.74114513563435	0.72813916684875
N	33.00957550400078	-25.57668513288526	5.13275466741538
N	34.66626440742905	-25.46653184457744	7.44795494572445
N	34.66733380718777	-27.68255411333032	4.05267420249684
C	32.60943069081706	-26.80549899115022	3.05469356456752
C	32.86440672165278	-23.90403800823859	6.90818506859174
C	36.56888868948050	-26.52584944120909	8.56397365466214
C	36.79388085058852	-28.85450344217294	4.33658672043113
C	30.51231405964403	-22.77806118807684	5.22729859667589
C	33.62721919945650	-22.58060232504242	9.61203473693637
C	39.07813076189633	-28.32645049509120	8.79259955544084
C	36.16121695624052	-30.02573165424446	1.52844680436675
C	32.31220493127477	-25.81313797356008	3.98633401444498
C	33.88940271778342	-24.37989324032100	7.72251109289161
C	36.95692682512855	-27.40624668447111	7.55702331712042
C	35.64325568837718	-28.53183820671749	3.62122388632108
C	31.24486050934939	-24.83044188527093	3.82727802512257
C	34.27011264113955	-23.79115777412290	9.00098314660381
C	38.15662023252637	-28.23236460849228	7.61197139131186
C	35.30768358849707	-29.06882766135187	2.30915980641014
C	31.34211206845837	-23.98361753040835	4.89755244926204
C	35.29607240124034	-24.55693220113292	9.48492221671949
C	38.25234918622299	-28.85069084599914	6.39442972097327
C	34.09556722331121	-28.52721713659096	1.97183828147054
C	32.45332699829992	-24.47252220619669	5.70506347844117
C	35.53874294586360	-25.59190623550385	8.48690932008055
C	37.09199179002713	-28.42021422432124	5.62538705366903
C	33.72379302080821	-27.64203824441562	3.06879918697422
N	36.33019343636462	-27.55366518104460	6.35426911654828

Fe	34.62818614916112	-26.61772979372624	5.77792131220892
C	34.71778071262163	-31.34291415801468	6.18410482261073
C	33.78300019649422	-32.09963242736363	5.24604253197651
C	32.13970512595046	-27.45257470587759	7.36316500532164
C	33.40853638834459	-27.92403185807519	6.69623641738367
C	33.52961093120289	-29.37974310312480	6.83714219919367
O	32.83328999408403	-30.10595825424378	7.54626978373079
O	34.53736979876162	-29.93270186872705	6.08555031657812
H	29.73297464743278	-22.60667335319114	4.47644119849637
H	31.12274745718710	-21.86566166986865	5.27908837619303
H	30.01089987224675	-22.88024399828035	6.19994891347606
H	30.79801388191110	-24.63707797408570	1.71818965029241
H	29.71210695329857	-25.72300071972145	2.58678466593126
H	29.55746692757954	-23.97387115348556	2.78851805108398
H	33.09155951605378	-27.79712445050845	0.19960133333770
H	33.79470133516008	-29.40961709119339	0.02624851775614
H	32.30386111511149	-29.18570453146901	0.95049917380638
H	35.71630174917451	-30.25793793142897	0.55428225324121
H	37.16450771706756	-29.61815830260263	1.34041282297789
H	36.30057537153252	-30.97815198669434	2.05880660512093
H	34.09254046707758	-22.31955952022652	10.56916461135295
H	32.55576703777961	-22.73754436611167	9.80039103858943
H	33.70901248509861	-21.70196389320328	8.95697404398671
H	37.14118216821965	-24.19520619018974	10.55492350652053
H	36.03794144784040	-25.29661118862573	11.37973078822477
H	39.90373103146460	-29.02181492662871	8.60495412180617
H	39.52098958172636	-27.35281389403541	9.04598288841112
H	38.55203397946396	-28.67838482671310	9.69085551641061
H	38.88855359143738	-30.76656859337527	5.61079772506961
H	39.82019537760192	-29.39542763373014	5.00633489252552
H	40.07562922633264	-29.97778820875375	6.65583662470848
H	35.69799290910049	-23.56179581419801	11.35781128094908
H	33.88561425145635	-31.72557928520728	4.22345328762457
H	34.01300370908263	-33.17222733215326	5.24919224845430
H	32.74648283103169	-31.96785703685060	5.56138294952862
H	34.56380147206728	-31.66334293182188	7.21756480564773
H	35.76305620931795	-31.50808415532606	5.90919908633223
H	32.18011385455567	-26.40194942174767	7.64333970062042
H	31.29187594326071	-27.56074401033682	6.66643369427132
H	31.88635665359809	-28.05620132829003	8.24123009080402
H	31.95351857849063	-26.87913016794881	2.19175251416451
H	37.17666115156639	-26.51215024163753	9.46422389990257
H	37.49923266951269	-29.53279318620454	3.86476044825838
H	32.32676207242093	-23.02482524234172	7.25094026054365
O	35.67509892148675	-25.31130520021345	4.93102542203332
H	36.42661318154255	-25.74771381224391	4.50276599676948

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B3LYP Scan/Melmid IPC Model/RKS/1.7 Angstrom Fe-C Bond Length Constrained Optimization

C	38.93005182900010	-22.86431629807447	5.02636104298103
C	37.75103115197995	-23.74903465052325	4.78443775503486
C	37.05029194606300	-24.59832160786372	5.60351849294821
N	37.11837801011115	-23.85517954647998	3.55363907269284
C	36.09126388716735	-24.74138320452435	3.68063606305197
N	36.02701566078537	-25.20597174888159	4.90818655568844
C	30.62311512952104	-24.45698063272235	2.27783158293010
C	35.52276355519083	-24.89700940293084	10.92148340418410
C	39.00964795910930	-30.14822631071505	6.03421107372566
C	33.61720038617337	-28.47391509121462	0.38700539397109
N	33.11111118662638	-25.50187129248735	4.89324209726739
N	34.51730719152476	-25.62791039709076	7.37598382757236
N	34.74225863269667	-27.60672766413788	3.86585175872213
C	32.85067013270876	-26.56961113853872	2.70596192888136
C	32.82395910106960	-23.96394023631898	6.77641170531886
C	36.22457046162417	-26.85787991384516	8.62900149688145
C	36.71061405718950	-28.98705434030690	4.31850843091948
C	30.65969038004834	-22.65629788207687	4.99106142375246
C	33.29882300628324	-22.89177521843779	9.64335853986686

C	38.61662622429626	-28.79397050461932	8.97285712353042
C	36.27661985938312	-30.02400628805798	1.43229236971618
C	32.50230093564615	-25.63102028123437	3.67360515836200
C	33.73929943257378	-24.53705265977316	7.65498792891844
C	36.66668382791342	-27.69733660285975	7.61094865006712
C	35.68111550924844	-28.53263127459074	3.50192515928165
C	31.48259368310171	-24.60668709747167	3.49816378696028
C	33.97792374277498	-24.07189191905863	9.01328131130707
C	37.80591630054710	-28.59632188149659	7.72584409292716
C	35.44038900486689	-29.00312962874038	2.14562711016853
C	31.49993865478162	-23.84760254086991	4.63713083609966
C	34.91261711138086	-24.91534075275996	9.55117892970640
C	37.97181115407191	-29.16643645857327	6.49191070012968
C	34.32233583442829	-28.34992422787217	1.70473387753958
C	32.52108284291150	-24.42523843536244	5.49910497116681
C	35.24517481381123	-25.87599201861420	8.50972220634372
C	36.91747358063347	-28.62536200619683	5.64615748955446
C	33.90581845815452	-27.47311801753312	2.78957479293961
N	36.14676907276639	-27.73840398057923	6.34503821633538
Fe	34.53968136919074	-26.71278111923359	5.66738142878358
C	34.07074051835048	-31.33473880987606	7.33151476386967
C	35.35190354832804	-31.89097499732675	6.73441600662609
C	32.09686208553205	-27.55509920024931	6.92570279546230
C	33.41252196293222	-27.84437657372248	6.24962141759325
C	33.55948006655924	-29.33728057162882	6.12689955310935
O	33.22275131671743	-29.97901771078838	5.16001933703364
O	34.02465813228878	-29.88801042756164	7.27305646341419
H	29.95196909793648	-22.41153641345096	4.19272154430826
H	31.27293581714870	-21.76284535185592	5.17049863913540
H	30.07402832142312	-22.83041044647534	5.90373415271979
H	31.22358035073407	-24.27837054742314	1.37540410239888
H	30.02474365163953	-25.35852927901532	2.08965311819518
H	29.92728638110587	-23.61814805853560	2.37747599499279
H	33.49624569221257	-27.49981999341686	-0.10551587996368
H	34.16734608452919	-29.12175907870382	-0.30258637327423
H	32.61189431734171	-28.90009818907640	0.50554607259045
H	35.96979601056426	-30.13396803972931	0.38732031529787
H	37.34077614429272	-29.75340916669077	1.43400191061476
H	36.19618251689260	-31.01406436826636	1.90123180910324
H	33.66628971205495	-22.71291092523456	10.65870233750625
H	32.21163588597858	-23.03446038013580	9.70918402339600
H	33.46598420481746	-21.97199127543842	9.06684336863107
H	36.61506945791267	-24.78996861986715	10.87871877439437
H	35.31486889469451	-25.82456359740019	11.47173325043137
H	39.43234040640422	-29.50580486123836	8.81242127537463
H	39.06582599665896	-27.85381291437500	9.32064951544692
H	38.00356418252657	-29.17958697667165	9.79855517906620
H	38.55957510280864	-31.09958214359423	5.71963705168760
H	39.57838946131784	-29.76391435234378	5.17705225191740
H	39.72839401482700	-30.37489449195980	6.82822054750983
H	35.13620032277199	-24.06770264593538	11.52210105082483
H	39.78734703612137	-23.13348727482302	4.39449613954175
H	38.70011263748319	-21.80642577293099	4.83955992206267
H	39.24810867517420	-22.95315456483275	6.06920410079543
H	36.22651016903415	-31.45373864956203	7.22065085557503
H	35.38326418488464	-32.97737066400674	6.86926284639001
H	35.40528166352590	-31.67362149030074	5.66694316308776
H	33.19260600944869	-31.73347253586914	6.82042705579678
H	33.99861722782187	-31.55831472493319	8.39729611528611
H	31.91349911879557	-26.49639443525492	7.08226997386398
H	31.27965702516717	-27.96810396513645	6.31762656001453
H	32.05750379562823	-28.07335181925641	7.89290139793954
H	37.37341960879958	-23.36332643573404	2.70939670751692
H	37.21667307769094	-24.81207461426550	6.64910422743698
H	35.43024514526488	-25.01486617336353	2.87124499366151
H	32.27669608488510	-26.56487144706803	1.78463171909197
H	36.72845183079894	-26.93732049189194	9.58717382665177
H	37.39336504993622	-29.71605613493218	3.89372297653891

H 32.27353113888012 -23.09895003118171 7.13269894910604

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B3LYP Scan/Melmid IPC Model/RKS/1.9 Angstrom Fe-C Bond Length Constrained Optimization

C	38.97957131291827	-22.87501802231093	4.99836677825344
C	37.78832306200740	-23.74506978873367	4.76402192735704
C	37.09375072103899	-24.59696506619566	5.58436870317170
N	37.13579756718308	-23.83039433459556	3.54194517093234
C	36.10259429866042	-24.70683317491180	3.67101922365402
N	36.05417290579261	-25.18557377209053	4.89529298802730
C	30.69549858536039	-24.39156927073389	2.24300265488105
C	35.57553127829636	-24.81861297868751	10.89983533701658
C	39.05089030815525	-30.11223679008743	6.04128015531013
C	33.66369008272702	-28.44242245326247	0.38028187334500
N	33.18345212288983	-25.42500504267236	4.86344834895424
N	34.58725156069971	-25.54362486770196	7.34801262667980
N	34.80741032756276	-27.55008679968015	3.84645626487472
C	32.92468497793499	-26.50287998903589	2.68000631118810
C	32.88517839348600	-23.88942956718368	6.74723468896894
C	36.29202565891941	-26.77370964691088	8.60503165906623
C	36.76292436971785	-28.94376858060390	4.31167664016062
C	30.71703936625591	-22.59202764925753	4.95663969671437
C	33.34406803868163	-22.82264094215225	9.62090874076876
C	38.66358748995160	-28.73361203186536	8.96861584283824
C	36.30574192270880	-30.01426657818977	1.43739782120407
C	32.57723726625563	-25.55814038428595	3.64296903326592
C	33.80202907453603	-24.45826175875896	7.62759032456637
C	36.73210353827174	-27.62135994840698	7.59186502320084
C	35.73525252530172	-28.49002977106587	3.49113588571480
C	31.55365925984091	-24.53736836669246	3.46481258337698
C	34.03353113341413	-23.99557461555911	8.98852662049946
C	37.86074157584277	-28.53330750515768	7.71696158803047
C	35.48527043229875	-28.97354481850143	2.14036906965508
C	31.56460206378317	-23.77866181406178	4.60412355725545
C	34.97155094487084	-24.83498611192703	9.52674879410357
C	38.02294225417872	-29.11492487989232	6.48796394568451
C	34.37472072618832	-28.31120150965103	1.69415151070406
C	32.58696011273314	-24.35156494654571	5.46848172098725
C	35.31270510870183	-25.79117436530055	8.48311443000137
C	36.97628777177187	-28.56833264083101	5.63524390384861
C	33.97116905182983	-27.41685829740609	2.77036608656850
N	36.21569263068708	-27.66609919912912	6.32490907356792
Fe	34.63722839539670	-26.61153422631143	5.62818785257865
C	34.11984064971094	-31.35763024387229	7.24749372300305
C	35.39925457151041	-31.86406884849068	6.60602370906053
C	32.07371033975243	-27.52358065735114	6.94572736587922
C	33.36623233483255	-27.86267808179274	6.28332757682238
C	33.50949884424223	-29.33548874178179	6.13428938961258
O	33.13158292100545	-29.94306609078383	5.15886807135820
O	34.04479900306690	-29.90958656653083	7.23337809153905
H	30.00772221982697	-22.35222362361821	4.15813503297801
H	31.32468422694039	-21.69453981838307	5.13534760581219
H	30.13243190443660	-22.76841040933934	5.86959526966311
H	31.29665657005610	-24.21249355084263	1.34106403262968
H	30.09971614025773	-25.29486648870408	2.05471481417997
H	29.99728297270699	-23.55438815864569	2.34045348439807
H	33.55552333744589	-27.47331217747989	-0.12510228549289
H	34.20183846578147	-29.10757422997031	-0.30229151554339
H	32.65240114096164	-28.85171397655612	0.50746262365214
H	35.99323011355995	-30.13432457788959	0.39518314968332
H	37.37325539971309	-29.75707627444651	1.43119861410169
H	36.21538045066584	-30.99716677270263	1.91956614372983
H	33.70414296745373	-22.64713846259639	10.63953828257899
H	32.25723555840416	-22.97144236462177	9.67920831868891
H	33.50942089936875	-21.89865351079030	9.05053078562080
H	36.66742129436390	-24.70487296986893	10.86272088555737
H	35.37100680680116	-25.74969735373460	11.44549958141157
H	39.47405601117946	-29.45291716215420	8.81476983659111

H	39.11908149423081	-27.79627730280244	9.31596782550482
H	38.04325781510932	-29.11131062091590	9.79266487625296
H	38.59170030493024	-31.06019593917249	5.72950635450889
H	39.62889963720664	-29.74030228807118	5.18477267548824
H	39.76281312002513	-30.34299727113515	6.84031835256149
H	35.18128917942097	-23.99420125097383	11.50228004237771
H	39.82475156335515	-23.14688083793832	4.35165543202624
H	38.75756702411056	-21.81317572959064	4.82544281475061
H	39.31117599808908	-22.97790179080350	6.03562512349364
H	36.27330430629894	-31.42036465493886	7.08697590145809
H	35.45876532123489	-32.95299804646182	6.70612227795970
H	35.42425603438925	-31.61205057913255	5.54504080312441
H	33.23860303443645	-31.75822018878420	6.74374157600700
H	34.07604936220796	-31.61360029089527	8.30737115922277
H	31.92405693290781	-26.45550589753138	7.07471712204683
H	31.24403434608677	-27.93222294196024	6.34951094430832
H	32.01457463065287	-28.02208110023653	7.92433226438495
H	37.38202473734294	-23.33063049653166	2.69985095109849
H	37.27266782132769	-24.82533542010950	6.62420960073768
H	35.42585054131300	-24.96400355802334	2.86996903702318
H	32.35113049440758	-26.50030217224263	1.75829803474429
H	36.79290646254440	-26.85263361252225	9.56493527205351
H	37.43845726967442	-29.68364074848818	3.89392276639929
H	32.32941886779979	-23.02749944944179	7.10296927597468

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B3LYP Scan/Melmid IPC Model/RKS/2.0 Angstrom Fe-C Bond Length Constrained Optimization

C	39.00570079252240	-22.86428824475840	4.98443169875452
C	37.81211602281090	-23.73141044603655	4.75138078117237
C	37.11931090796057	-24.58412507871839	5.57192807694038
N	37.15536522565881	-23.81192734344492	3.53132822682903
C	36.12097035735017	-24.68629797145719	3.66009324795457
N	36.07620103261922	-25.16851356929973	4.88378247627727
C	30.73420137172903	-24.35416363147445	2.22360444916172
C	35.60456464896859	-24.78532803891751	10.88726138184993
C	39.06979462571572	-30.09782204029044	6.03767937803316
C	33.69176237394178	-28.41753814818487	0.36867998416063
N	33.21816662516252	-25.39032997159382	4.84720125328702
N	34.62192015605368	-25.50773837139198	7.33311456139453
N	34.83735385696008	-27.52294823552407	3.83382081185875
C	32.96278473925224	-26.46646855754499	2.66225433181732
C	32.91312298763452	-23.85965194544375	6.73423598543304
C	36.32840336530798	-26.73557329738091	8.59010463741524
C	36.78409760659037	-28.92675506957376	4.30541573816341
C	30.74477391388096	-22.56307027523401	4.94263602670837
C	33.36399924712278	-22.79764374455880	9.61147832556914
C	38.69184494623823	-28.70511234786821	8.95915331997878
C	36.31929498534427	-30.00743640625400	1.43505250529739
C	32.61486110054415	-25.52135797676775	3.62500565680680
C	33.83141974478634	-24.42662594489845	7.61451565657855
C	36.76591723257460	-27.58716541326945	7.57876884668142
C	35.75874414446739	-28.47086559555174	3.48277610380901
C	31.58977146925795	-24.50181903170558	3.44703066061590
C	34.05982771333391	-23.96555709274061	8.97673668808967
C	37.88962058787483	-28.50508153145043	7.70705902264383
C	35.50643364360852	-28.95760404675814	2.13335045230260
C	31.59615296377862	-23.74656687508115	4.58867606080705
C	35.00175582834525	-24.80137047154460	9.51364886716014
C	38.04706190730383	-29.09343222908527	6.48064780366966
C	34.40207886805950	-28.28766275800307	1.68308847271457
C	32.61799606257604	-24.31965459046826	5.45373708345683
C	35.34777670866166	-25.75408614282470	8.46817318118774
C	37.00229610082145	-28.54480419054554	5.62655585389372
C	34.00404491448916	-27.38647295631261	2.75590256327806
N	36.24795891289875	-27.63457606264867	6.31259144951535
Fe	34.68344964310003	-26.56569743973236	5.60718191300201
C	34.13785120682957	-31.36544205020775	7.23439849842550
C	35.41598650446649	-31.84653654313963	6.57204773856213

C	32.05193066798414	-27.51272234004838	6.94496052291835
C	33.33992871404554	-27.87561699912714	6.29932515358955
C	33.48458082786970	-29.34105718440819	6.15123133898339
O	33.09609342599401	-29.93872018020529	5.17277751890697
O	34.04394223016650	-29.91759827817574	7.23482685635154
H	30.03618927977956	-22.32307594855971	4.14350641967729
H	31.34969709061250	-21.66439442916950	5.12470116842073
H	30.15901430417959	-22.74308233330878	5.85417384252784
H	31.33714339586313	-24.17146402842645	1.32355095817226
H	30.14045213906684	-25.25795106285849	2.03116655583441
H	30.03423804217654	-23.51848680713202	2.32168228949915
H	33.59350354036589	-27.44946801423624	-0.14079544631608
H	34.22455184263722	-29.09048934230804	-0.31045371749109
H	32.67636364197016	-28.81662388143392	0.49579541275481
H	36.00643198185200	-30.12937195319473	0.39314089833134
H	37.38872274057856	-29.75826518555636	1.42832224948758
H	36.22157335903420	-30.98777533641044	1.92104221489247
H	33.72132373164786	-22.62359444466928	10.63134940927005
H	32.27768713171644	-22.95128436169047	9.66724406060354
H	33.52625058638898	-21.87112868466207	9.04427997059450
H	36.69594200788229	-24.66617568824418	10.85140677186699
H	35.40431230260379	-25.71875304548278	11.43057713973004
H	39.49933506874203	-29.42821718096623	8.80734307750294
H	39.15126662621350	-27.76870890628660	9.30388590996252
H	38.07016292993838	-29.07789626708223	9.78446932731149
H	38.60642384612797	-31.04469232645738	5.72876109157573
H	39.65000640255201	-29.73184902745536	5.18004561101352
H	39.78036235426929	-30.32942063181109	6.83771233804626
H	35.20581613735994	-23.96436217844616	11.49147140752171
H	39.84842747508315	-23.13645306163735	4.33469880873553
H	38.78514830375364	-21.8016831772354	4.81455044162006
H	39.33994464915768	-22.97024562290319	6.02051349717312
H	36.28876359406760	-31.39169692154175	7.04464852430429
H	35.49425418036748	-32.93504111606985	6.66316604452987
H	35.42255323905452	-31.58599662888392	5.51284152999935
H	33.25547324762557	-31.77285608028376	6.73823090837612
H	34.11064813226211	-31.63115800898485	8.29231500762716
H	31.91198275342037	-26.44080648237924	7.05222484237084
H	31.22268045936393	-27.92819079948530	6.35197114773733
H	31.98103795021803	-27.99442333958532	7.93202983618304
H	37.39944542887329	-23.31013938317080	2.68987106923983
H	37.30099264589443	-24.81566038913791	6.61037063219011
H	35.44087511881814	-24.93952635411058	2.86088253936384
H	32.39143922706532	-26.46187280182779	1.73913305779527
H	36.82975779997491	-26.81331885847632	9.54990553974735
H	37.45499256271164	-29.67258928517579	3.89067844958839
H	32.35399421806535	-23.00034469312182	7.09118742062135

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B3LYP Scan/Melmid IPC Model/RKS/2.1 Angstrom Fe-C Bond Length Constrained Optimization

C	39.03741736348959	-22.84844442966516	4.96820669553000
C	37.84122817328321	-23.71225787077907	4.73646402094906
C	37.15050960334347	-24.56652421856573	5.55678612545107
N	37.17938420509405	-23.78657927306368	3.51885082145446
C	36.14367023655191	-24.65887772261742	3.64737417888571
N	36.10325683470100	-25.14587125587251	4.86991548325103
C	30.76919849457621	-24.31900992827923	2.20637816808973
C	35.63654319811978	-24.75431087218311	10.87293934643065
C	39.08404843663633	-30.08927374001961	6.03175784479710
C	33.72215049920147	-28.38778260603023	0.35325368458424
N	33.25293493942578	-25.35660545168275	4.83015754707594
N	34.65738891732561	-25.47429189354817	7.31697859638201
N	34.86837795157223	-27.49372722438837	3.81875164951195
C	33.00093029384728	-26.42902282639775	2.64291864489941
C	32.93982762650035	-23.83347003240670	6.72219462976188
C	36.36604249183270	-26.69961355391291	8.57321326224018
C	36.80466650769567	-28.90986909201063	4.29637758906191
C	30.76821869632467	-22.53895016993996	4.93246617402854

C	33.38441322812977	-22.77644819108999	9.60239888967994
C	38.71955705290971	-28.68047844191343	8.94678478217304
C	36.33483334728244	-29.99609730440532	1.42839780278074
C	32.65170513092231	-25.48506891813794	3.60657062593664
C	33.86088386197625	-24.3980837773007	7.60122919672390
C	36.79995903591042	-27.55495483881439	7.56333572887546
C	35.78306438368504	-28.44957835168595	3.47134973587098
C	31.62353807179511	-24.46818778803410	3.43049956223436
C	34.08692395478064	-23.93868351500040	8.96454400918041
C	37.91752728774594	-28.48009697050831	7.69459557716095
C	35.52923701608337	-28.93798727054006	2.12264604676749
C	31.62504892060816	-23.71754737554303	4.57523133243216
C	35.03375350097551	-24.77026202736644	9.49930617997875
C	38.06893445171963	-29.07548943206009	6.47083809897192
C	34.43117423558987	-28.26031438655520	1.66860231271045
C	32.64776444022738	-24.29018797934412	5.43964606599714
C	35.38422485914141	-25.71916202546635	8.45171004733509
C	37.02706719216012	-28.52301330958036	5.61548090640849
C	34.03812960706178	-27.35362190635344	2.73881459903128
N	36.28002992442124	-27.60383544775861	6.29789933496702
Fe	34.72997792280733	-26.51995044596232	5.58442831118832
C	34.14886101104661	-31.37091829162390	7.23227889216254
C	35.43459338471258	-31.82323913450409	6.56506591624952
C	32.02593871875041	-27.50321023663998	6.93409706314679
C	33.31286963798264	-27.88873304419711	6.31122835569670
C	33.45963059841269	-29.34785142589511	6.16967213353648
O	33.06958967792904	-29.93814524706357	5.18620993616596
O	34.03209695447583	-29.92395592157946	7.24465377026413
H	30.05909465367998	-22.29938715111885	4.13365970774677
H	31.36899984553707	-21.63817038975215	5.11793888458384
H	30.18261248735842	-22.72434990208369	5.84305259352909
H	31.37274639740088	-24.13061540735104	1.30787484197218
H	30.17905144470349	-25.22420574830728	2.00941398711799
H	30.06600151197317	-23.48627525000507	2.30654551542773
H	33.63285881451131	-27.42022882449741	-0.15890167921395
H	34.25052649722888	-29.06688471579115	-0.32321922223513
H	32.70315215888669	-28.77803591061198	0.47930340439805
H	36.02338670605082	-30.11757373685955	0.38598326518204
H	37.40630259396636	-29.75580503922491	1.42354079537553
H	36.22808485589679	-30.97467700698649	1.91606848365305
H	33.73978262083487	-22.60378305117352	10.62321125642693
H	32.29882766685873	-22.93581790404228	9.65657611738100
H	33.54230360108095	-21.84720662152409	9.03840812254019
H	36.72725249662848	-24.62888355889175	10.83741316772622
H	35.44177654887667	-25.69028192346996	11.41392331793678
H	39.52115649309951	-29.41068587661536	8.79765620292441
H	39.18692781183248	-27.74613860484462	9.28647389114771
H	38.09603527356384	-29.04424065140816	9.77475927178690
H	38.61346011242298	-31.03236470715587	5.72214074517077
H	39.67039333886751	-29.72950818856280	5.17559926884481
H	39.79002447690135	-30.32647935241813	6.83422914720671
H	35.23319864151989	-23.93721373617431	11.47936503674514
H	39.87674353348358	-23.11948275298400	4.31365479753200
H	38.81802059692059	-21.78475124815235	4.80384535527701
H	39.37586850955879	-22.95952665387085	6.00236686338674
H	36.29902258562905	-31.35380484419119	7.03863390418388
H	35.53418155648377	-32.91051156172887	6.64951481867844
H	35.43430601554910	-31.55598246700111	5.50748884627653
H	33.27278778850268	-31.78821629261554	6.73328774997334
H	34.12635225227324	-31.64522817278249	8.28800536623541
H	31.89483393347218	-26.42829479842165	7.02269260884287
H	31.20042726003044	-27.92306293517623	6.33805396272199
H	31.93660483507432	-27.97182234888015	7.92675563972019
H	37.42096634559685	-23.28193741927324	2.67843893186237
H	37.33575173250849	-24.80243959111537	6.59344934262150
H	35.45969257734473	-24.90725839200824	2.85015799099956
H	32.43120930554387	-26.42259446952687	1.71875455618727
H	36.86797707133780	-26.77681615523953	9.53280014770985

H	37.47039833439800	-29.66187408492257	3.88438233754465
H	32.37677194184563	-22.97762303852214	7.08143235085984

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B3LYP Scan/Melmid IPC Model/RKS/2.2 Angstrom Fe-C Bond Length Constrained Optimization

C	39.07413295927638	-22.82437138459348	4.96504789323975
C	37.87692140271239	-23.68536839712462	4.72833483031321
C	37.18632931363296	-24.54401962196400	5.54386575980024
N	37.21419930207444	-23.75102970689698	3.51079317760309
C	36.17746801237202	-24.62259774528613	3.63361847446110
N	36.13767543592720	-25.11754038550298	4.85349592709507
C	30.80984492761280	-24.26820572614739	2.18524906134559
C	35.66448387862947	-24.74347170122949	10.85787285863151
C	39.09414348253957	-30.08592854612037	6.00844586983583
C	33.74533462814320	-28.35017490385398	0.32837912070240
N	33.29201398914390	-25.31803573279116	4.80643612152733
N	34.69065665429023	-25.44828869023755	7.29677202454623
N	34.90096212730946	-27.45659177535009	3.79111077688929
C	33.04412509654754	-26.37747881304729	2.61225312379524
C	32.96355524225798	-23.81430983697480	6.71211087840302
C	36.40490439782612	-26.67137352756330	8.54781126057072
C	36.81946962780213	-28.89486002349000	4.27534361356920
C	30.79140855270685	-22.51426094882072	4.92808794769936
C	33.39519919064112	-22.77645666624552	9.60113918122987
C	38.75405385908925	-28.65854325690799	8.91744846764867
C	36.33387537055764	-29.99145994430088	1.41441047553093
C	32.69427608895261	-25.43771610194422	3.58005878759769
C	33.88603284301625	-24.37995012135874	7.58849517559847
C	36.83543772113612	-27.52723008235695	7.53691924001231
C	35.80309695784271	-28.42621571846159	3.44849499887542
C	31.66224270928631	-24.42387736797101	3.40990286811835
C	34.10753522450383	-23.92819154495211	8.95516859922208
C	37.94801787292467	-28.45853826689646	7.66767061131449
C	35.54350856745157	-28.91756851796842	2.10177273502020
C	31.65617796488959	-23.68429367008410	4.56185231957352
C	35.06140771934766	-24.75518492926815	9.48428888399989
C	38.09006603158646	-29.06062627094811	6.44603170010237
C	34.45593434922506	-28.22632820273324	1.64323360323952
C	32.67913445564162	-24.25999310151587	5.42390627131884
C	35.41912105340872	-25.69442365477867	8.43042469875036
C	37.04876173904393	-28.50438917400878	5.59233823974037
C	34.07401288879414	-27.30997786098274	2.70935673797329
N	36.31034947090451	-27.57684473264413	6.27355613955407
Fe	34.77830686287114	-26.47464765110796	5.55254380085420
C	34.16253832827294	-31.35900393933636	7.27937892952201
C	35.47012774356486	-31.78503990043795	6.63838910838449
C	31.98025131752053	-27.50105069915234	6.86376049363352
C	33.28221315228583	-27.90566666921559	6.29678043588582
C	33.44691652060307	-29.35932600160206	6.19220363794151
O	33.08009884768843	-29.95981656073451	5.20445111823681
O	34.01287813489143	-29.91430146851081	7.27907130421081
H	30.08290944518418	-22.27127390827761	4.12975101722597
H	31.38636021994462	-21.61174687998489	5.12372686789608
H	30.20454822513234	-22.71162280416224	5.83537721315119
H	31.41429155524926	-24.06852466639555	1.28977834131180
H	30.22496353618723	-25.17472881984496	1.97879373358603
H	30.10192900462217	-23.44019815148601	2.29133814636848
H	33.67799254628332	-27.38563934167005	-0.19289193179730
H	34.25886771240442	-29.04715324870918	-0.34125868807592
H	32.71771161280090	-28.71625134574396	0.45699781965692
H	36.00898869292934	-30.12751145070794	0.37793727131548
H	37.40686840865630	-29.75839252281740	1.39290291806842
H	36.22685670116206	-30.96117809868397	1.91932470592598
H	33.74430006511080	-22.61204296330761	10.62550321775682
H	32.31026200755910	-22.94238961615428	9.64808048349664
H	33.55060178567164	-21.84054647659637	9.04753288839103
H	36.75347989665718	-24.60329564715845	10.82313544428889
H	35.48262599391015	-25.68671803437546	11.39068032287049

H	39.55738025868668	-29.38619546439676	8.76499410085782
H	39.21958300671279	-27.72331251821681	9.25710757387665
H	38.13427339599411	-29.02526030943315	9.74701167421414
H	38.61427043265829	-31.03036197234567	5.71742319573228
H	39.67199275479599	-29.74151089277209	5.14036526867999
H	39.80851237173089	-30.31641461309513	6.80548256806843
H	35.25079853678295	-23.93718089010304	11.47176799440218
H	39.91345975486811	-23.09337612078173	4.30968513962888
H	38.85611060582917	-21.75965106474802	4.80575617605742
H	39.41173232907263	-22.94093738524056	5.99886288039068
H	36.31450058813956	-31.29019173287984	7.12197859939407
H	35.59447104209127	-32.86872069406660	6.73467368117362
H	35.48220094742899	-31.52718466732169	5.57849345776494
H	33.30488084914424	-31.79966566560133	6.76878945479825
H	34.12758295946633	-31.62569243222270	8.33663156685681
H	31.80440835750213	-26.42939248768187	6.81997995777762
H	31.16007966445206	-28.04087942033324	6.36720516081865
H	31.94874108540822	-27.83013848033934	7.91640057292661
H	37.45556612482670	-23.24126334940411	2.67348894328467
H	37.37204716995885	-24.78667431921189	6.57874930250625
H	35.49246448236714	-24.86485763960406	2.83557168751917
H	32.47626440528546	-26.36584846356021	1.68694593960864
H	36.90875423530801	-26.74926407509152	9.50638679940952
H	37.47669540709000	-29.65546505523139	3.86530700941545
H	32.39404763418414	-22.96525734081853	7.07736750228158

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B3LYP Scan/Melmid IPC Model/RKS/2.3 Angstrom Fe-C Bond Length Constrained Optimization

C	39.09965978940421	-22.79934489982942	4.94959997175890
C	37.90362152241986	-23.66131447689633	4.71037893179441
C	37.21377404210627	-24.52226523257223	5.52397177160002
N	37.24120029010819	-23.72432193862997	3.49270255226082
C	36.20479142405568	-24.59675558516415	3.61281017346499
N	36.16523050588280	-25.09464940801434	4.83195184353225
C	30.84370750990871	-24.25839285589895	2.14803428506664
C	35.67743383799204	-24.70570539286579	10.83546321465830
C	39.10855675601587	-30.07570333197613	6.01535630134904
C	33.82711812025840	-28.30029282197007	0.28519062756303
N	33.31959109871499	-25.30156569790065	4.77893406822017
N	34.71557877262473	-25.41880817572865	7.27194598508277
N	34.93076538672235	-27.43800610015216	3.77410858931929
C	33.08972865562689	-26.35185307112142	2.57843912137224
C	32.97545800629683	-23.79992729709678	6.68497185083312
C	36.42834404964817	-26.63694418305374	8.53123240754536
C	36.84512451229710	-28.87932227625703	4.26993080432838
C	30.79503740982206	-22.51718232947156	4.89801819426092
C	33.39611629187957	-22.75538168052069	9.57365967056937
C	38.76266157775270	-28.63939109677077	8.91819019252367
C	36.39825207797738	-29.95291238326421	1.39448135880446
C	32.72865184791448	-25.41942522649760	3.54879416662945
C	33.90285756123986	-24.35562335157327	7.56235260294250
C	36.85816248675356	-27.49898528792691	7.52533185026076
C	35.83683088047813	-28.40652740435411	3.43564414294684
C	31.68970437987160	-24.41295292597675	3.37731648928690
C	34.11786406801669	-23.90224662479452	8.92943919877559
C	37.96343549211445	-28.43790293602913	7.66442436617727
C	35.59530957802225	-28.88821464397843	2.08191106239045
C	31.67083527623027	-23.67913384015293	4.53260508573770
C	35.07658184279664	-24.72263570574585	9.46090264245213
C	38.10506809113748	-29.04674079720855	6.44632744272033
C	34.51498645398731	-28.19217213519008	1.61351018434203
C	32.69492722015828	-24.24961090728379	5.39729328099113
C	35.44267977503795	-25.66004045572831	8.40827395359933
C	37.07023174514664	-28.48662304321975	5.58680765254356
C	34.11905899314548	-27.28402972857836	2.68157421448099
N	36.33597819716996	-27.55048657531050	6.26055293526903
Fe	34.81621502493517	-26.43726038541535	5.52383533594421
C	34.15559332030565	-31.39658926173659	7.24253489850258

C	35.39716857608585	-31.83099536477202	6.48644446981978
C	32.06181482570546	-27.42464907006207	7.05813595188055
C	33.26671596621589	-27.91169012172289	6.36947688147726
C	33.37423197457217	-29.36287384192376	6.27633246177978
O	32.86594929094034	-29.93219963869688	5.33144003807936
O	34.04175525062742	-29.94763823655438	7.28237504488625
H	30.08575737656155	-22.28052988761512	4.09845116791874
H	31.38147201733493	-21.60928054946232	5.09459870624081
H	30.20840483579233	-22.71955794840846	5.80431368731294
H	31.451482444440068	-24.04018178653434	1.25905404577797
H	30.27493079104312	-25.17188684657813	1.92827487936168
H	30.12216867936025	-23.44262938511044	2.25681129108015
H	33.78014631452513	-27.33161912866437	-0.23076027612065
H	34.34546688166989	-28.99843265567785	-0.37955660844928
H	32.79327930014883	-28.65567427434749	0.39194526712819
H	36.09222264297287	-30.07479062070803	0.35053686431826
H	37.47107641402287	-29.71842748569042	1.39516908749473
H	36.28417310557695	-30.93001668304410	1.88337984609942
H	33.73681180232634	-22.59250514636771	10.60109152933799
H	32.31152618721193	-22.92576938945945	9.61188852661375
H	33.55153865061982	-21.81722992789227	9.02390623397710
H	36.76373719978717	-24.54523420022803	10.80283284268461
H	35.51274376054821	-25.65449958952136	11.36398843054144
H	39.56651225560212	-29.36721213081650	8.76928069432362
H	39.22680519515879	-27.70476230659607	9.26133968749097
H	38.13826328504355	-29.00675781753848	9.74408883633913
H	38.62926488385691	-31.01707494029026	5.71401476865802
H	39.69774028856532	-29.73001094092784	5.15527638579459
H	39.81310197314928	-30.31258894009299	6.81919827197258
H	35.24808961871099	-23.90996454830209	11.45231908521240
H	39.93878288299054	-23.06403792401882	4.29226131681990
H	38.87954477111894	-21.73433882305670	4.79514863712857
H	39.43847456470242	-22.91967280371935	5.98257550276692
H	36.28821235393438	-31.36525659154167	6.91202716789505
H	35.50616759808199	-32.91904151794974	6.54531050503715
H	35.32974323897782	-31.54637508576505	5.43511417152264
H	33.24944072812418	-31.80709494685460	6.79494089266617
H	34.20105089138939	-31.68544049316107	8.29336350725942
H	31.75323590683656	-26.43580899263591	6.71792785725840
H	31.21841110292315	-28.12531360512525	7.07724254622927
H	32.39739363987675	-27.29004639695349	8.10365100852580
H	37.48199904472493	-23.21199688113232	2.65685396706035
H	37.39975468471208	-24.76753144175458	6.55808670050339
H	35.51930489965191	-24.83631160338206	2.81445780278583
H	32.53102320258811	-26.33572067926732	1.64763795231972
H	36.92934054575970	-26.71239464934792	9.49155649848265
H	37.50285593009919	-29.64170833177124	3.86388810167713
H	32.39834884338879	-22.95531991109654	7.04869955512773

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B3LYP Scan/Melmid IPC Model/RKS/2.4 Angstrom Fe-C Bond Length Constrained Optimization

C	39.13299006612300	-22.76271983855491	4.94245071938230
C	37.93906491774538	-23.62607982551609	4.69792941862883
C	37.25092028044657	-24.49259367803209	5.50690758816641
N	37.27728317911101	-23.68410678076086	3.47965684922535
C	36.24242082935870	-24.55901074612594	3.59443080363488
N	36.20353176701433	-25.06345326388793	4.81133984891584
C	30.88501405857146	-24.21221550545461	2.12538244664546
C	35.70134366917183	-24.70200668717928	10.82041765017238
C	39.12309776287465	-30.07061847906688	5.98846930129798
C	33.85466927380465	-28.26276977126722	0.25778432333120
N	33.35623045804420	-25.27000405977568	4.75589120091606
N	34.74839423187908	-25.39810643971756	7.25034548471335
N	34.96428187638124	-27.40430179674230	3.74645412288624
C	33.13128216228084	-26.30711684533720	2.54875215522474
C	32.99878797825906	-23.78558382045035	6.67316618796552
C	36.46688179495998	-26.61309941335836	8.50421500483645
C	36.86493837759097	-28.86289649536242	4.24504491744890

C	30.82091061186788	-22.49502664837277	4.89009536843097
C	33.40408465852817	-22.76251520229113	9.57106587393808
C	38.79732954552149	-28.62014335386775	8.88674800934404
C	36.40690296823432	-29.94083290923227	1.37390511766671
C	32.76892522284983	-25.37919417172493	3.52298073573166
C	33.92717074704265	-24.34304486896004	7.54823242340354
C	36.89442188438777	-27.47384182996326	7.49645998200213
C	35.86064271027107	-28.38303967919355	3.41014611165922
C	31.72745116509790	-24.37468206786871	3.35611165797196
C	34.13634965964903	-23.89835402367903	8.91907669089436
C	37.99524091974180	-28.41802614124054	7.63484041249890
C	35.61492554208606	-28.86554547465930	2.05746832210713
C	31.70215382556785	-23.65066345911123	4.51745156859037
C	35.10188147505259	-24.71412635371897	9.44523736531938
C	38.12911896872195	-29.03186772838352	6.41835881507907
C	34.54277672597110	-28.15898803747564	1.58630450754977
C	32.72540789344103	-24.22471180413151	5.38068829002421
C	35.47646312699128	-25.64067358330602	8.38614096679464
C	37.09534769337740	-28.46788705502618	5.56024928494062
C	34.15527975045332	-27.24480745650990	2.65234239194958
N	36.36795040961649	-27.52486083001792	6.23302052197806
Fe	34.86439111350156	-26.39740855955777	5.49171655575741
C	34.16369405740276	-31.38610786882343	7.30767969745851
C	35.41839515411468	-31.79655758962758	6.55999901573075
C	32.02374000158741	-27.40832723766627	7.01179842464449
C	33.23772948130315	-27.92717780604984	6.37136306526230
C	33.35401728119982	-29.37414021963640	6.32315418282896
O	32.85770208868340	-29.95547592473834	5.37732095474769
O	34.01895323740353	-29.93922950374367	7.33979299387241
H	30.11100503960876	-22.25588851333878	4.09181171037439
H	31.40317090169016	-21.58590190638835	5.09334016934446
H	30.23466402826694	-22.70649512864597	5.79457258512281
H	31.49434044261298	-23.97565901783052	1.24209684979389
H	30.32652564958849	-25.12833493135328	1.89069490409300
H	30.15462484347431	-23.40539526794231	2.24199829581150
H	33.82002046555039	-27.29501284212465	-0.26089997299786
H	34.36486245151490	-28.96910402040963	-0.40461227250761
H	32.81637683913644	-28.60500889407496	0.36457837111755
H	36.09207415067756	-30.07127924203896	0.33360760696819
H	37.48099396281304	-29.71195633565690	1.36404455815724
H	36.29169598624129	-30.91244277906451	1.87335635892428
H	33.73343597123640	-22.61206841153627	10.60409343727169
H	32.31976809313836	-22.93687283603606	9.59577710882255
H	33.56199213330781	-21.81645492487124	9.03562340069860
H	36.78510650853229	-24.52441607257512	10.79031456901379
H	35.55096159064983	-25.65853949413654	11.33914214603301
H	39.60224224352259	-29.34630346728542	8.73521131542556
H	39.26021363717838	-27.68510411787664	9.23039556793225
H	38.17534973351658	-28.99007881796199	9.71340845544265
H	38.63638713930243	-31.01553982176657	5.71045164607453
H	39.69940015145953	-29.74049276415870	5.11379979279132
H	39.83974111452128	-30.29660452083654	6.78483545998752
H	35.25960331236386	-23.91919001181630	11.44503727961628
H	39.97369021889965	-23.02289216777622	4.28529159338369
H	38.91078634651433	-21.69756947122216	4.79193466742884
H	39.47045608155600	-22.88657202187360	5.97545662460680
H	36.29608712780931	-31.30586637514787	6.98524029407771
H	35.55311618715200	-32.88101508009920	6.62814824743394
H	35.34880733545413	-31.52173662100131	5.50620903154642
H	33.26818920919428	-31.81762847448929	6.85839404916834
H	34.21011617977154	-31.66851671892388	8.36010793190416
H	31.72058727503860	-26.43942537002974	6.61313317825198
H	31.18037361625503	-28.10676724922551	7.07213451109697
H	32.35974726256910	-27.20834185089166	8.04753274312057
H	37.51740857810086	-23.16710331696758	2.64653711250457
H	37.43675120898224	-24.74269397798875	6.53987833033551
H	35.55803537824193	-24.79647034202739	2.79453663012243
H	32.57442207781729	-26.28622014546066	1.61690193135129

H	36.96930974220647	-26.69003209715824	9.46370848638204
H	37.51568356815449	-29.63210165249964	3.84052977193150
H	32.41612882508787	-22.94715256841018	7.04243529447179

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B3LYP Scan/Melmid IPC Model/RKS/2.5 Angstrom Fe-C Bond Length Constrained Optimization

C	39.18328364685905	-22.72732404999376	4.95269738050506
C	37.98990188149011	-23.58770380543082	4.69535767455247
C	37.29855947497975	-24.46171794276203	5.49351077322133
N	37.33231155077474	-23.63292176553960	3.47441836004623
C	36.29623525200506	-24.50803531802484	3.57646584988338
N	36.25307048695760	-25.02467109558176	4.78850178721011
C	30.92142092689916	-24.16139985588591	2.10530723965489
C	35.71330881204724	-24.74915548016189	10.80729115496487
C	39.13900242955779	-30.07432863787577	5.92855422242592
C	33.88476543607239	-28.20564095607097	0.20890099104870
N	33.40249943760428	-25.23466149674317	4.72148348065364
N	34.78345366057530	-25.39423112169615	7.22073292211386
N	35.00857067006076	-27.35739488920743	3.69664180261198
C	33.18226542566735	-26.24645721834390	2.50216026364322
C	33.01753075472359	-23.79152885943926	6.66514085029776
C	36.51091256949558	-26.60888961401331	8.46203586355310
C	36.88976611301494	-28.84233790952474	4.19329974455106
C	30.83485934884860	-22.49074870767376	4.89737969283657
C	33.39171447000717	-22.82142314763319	9.58544975943947
C	38.83928692731575	-28.61984041583373	8.82788982754075
C	36.41420266364510	-29.91866154201593	1.32715352466735
C	32.81694026244849	-25.32974484950604	3.48585159390033
C	33.94683523232769	-24.35557454741831	7.53503161260564
C	36.93668592016783	-27.46141894331825	7.44706077821975
C	35.89184215509746	-28.34837922531003	3.35956192669894
C	31.76468442701200	-24.33484859902888	3.33411177689430
C	34.14383021481772	-23.93328635122134	8.91507953463984
C	38.03252964205520	-28.41212930365440	7.57985352812587
C	35.63904182729515	-28.82928363217806	2.00766669884743
C	31.72965965524889	-23.63021466320982	4.50767234190818
C	35.12033194787711	-24.74331607027002	9.42934171583549
C	38.15697196412021	-29.02599166074891	6.36236485367782
C	34.57677125345126	-28.10851687268591	1.53597189307851
C	32.75794197515353	-24.20650391608289	5.36252884771034
C	35.51155971831447	-25.64515814342777	8.35545165683761
C	37.12512908111211	-28.45229884530200	5.50872050701483
C	34.20153793294477	-27.18904855027074	2.60172227022621
N	36.40546334017033	-27.50487849868819	6.18490009643218
Fe	34.91855229603994	-26.35541903638797	5.44237488574519
C	34.20165341570158	-31.29529836080037	7.53089462245548
C	35.43451621987028	-31.73049168969265	6.76082952963015
C	31.93775369368073	-27.37413484937842	6.82865260240056
C	33.20012675155187	-27.93330097889202	6.34087486249636
C	33.35771799122941	-29.36680807718694	6.42784770215618
O	32.89077575434692	-30.01310390500162	5.50575395615527
O	34.02372947705988	-29.85140963003054	7.47976161245891
H	30.11647908461400	-22.25406862438178	4.10599210479003
H	31.40603638387112	-21.57553931710731	5.10490529718345
H	30.25780585106671	-22.71786383083539	5.80391340944287
H	31.52046609814027	-23.84881251440243	1.23850492885902
H	30.41685534987251	-25.09506624804976	1.82331538424818
H	30.14601836792674	-23.40330885567897	2.25409442248892
H	33.87414665554749	-27.24191950025802	-0.31837683167751
H	34.37566564064259	-28.93072392482197	-0.44770975342573
H	32.83811042603489	-28.51993783923009	0.31993125167814
H	36.08512228021300	-30.05961738014251	0.29268569841027
H	37.48992780257726	-29.69839441093127	1.30097585042498
H	36.29791355568692	-30.88263858809293	1.84082279391633
H	33.70968748643880	-22.69063081957872	10.62468736091375
H	32.30947992625100	-23.00909541753135	9.59596939395632
H	33.54285375645662	-21.86148690168682	9.07335051080092
H	36.79479127466674	-24.55691025310357	10.78591668899124

H	35.57295083064518	-25.71721376080383	11.30716852730522
H	39.62950296324442	-29.36199960052052	8.67665025376443
H	39.32239440804755	-27.69119198656077	9.16071767742089
H	38.21684987615671	-28.97132472732049	9.66197818632954
H	38.64054132737088	-31.01192716885173	5.64616717520002
H	39.72035863515136	-29.74800012822547	5.05565472453891
H	39.85209050309739	-30.31237834230432	6.72459569916495
H	35.25859270073924	-23.98410447818302	11.44441503825534
H	40.02459712446743	-22.97850129062425	4.29282221766784
H	38.96088464937795	-21.66030855819683	4.81626938181189
H	39.51985812749557	-22.86495627839279	5.98423835127603
H	36.32003909967971	-31.20229308310532	7.11978927043462
H	35.59009092821387	-32.80658140985990	6.89051406950600
H	35.31815404990586	-31.52447504897589	5.69574701863662
H	33.29904250850261	-31.77241253515809	7.14614308530841
H	34.29323256782433	-31.50763531479135	8.59655532373823
H	31.59581863053815	-26.54193448258599	6.20814154357510
H	31.13024662692592	-28.08508198726754	7.03816288931444
H	32.23371565801499	-26.89179197069871	7.77971098035283
H	37.57611536181671	-23.10820150518612	2.64725995275452
H	37.48030436184248	-24.72267641004617	6.52450183840501
H	35.61456433437538	-24.73761080950482	2.77201133763480
H	32.62597706372654	-26.21789532712866	1.57013113750446
H	37.01481038680075	-26.69275460415827	9.42016919617749
H	37.53057446546838	-29.61886053125018	3.78687890110130
H	32.42315471685877	-22.96728660331596	7.04753219424509

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B3LYP Scan/Thiolate IPC Model/RKS/1.7 Angstrom Fe-C Bond Length Constrained Optimization

C	30.79993486942871	-24.35999094127123	2.21132676192681
C	35.83599345156205	-24.87031072459656	10.77479203319471
C	39.01032667007517	-30.32905847018932	5.92198657786808
C	33.69517771586980	-28.38512945255116	0.27551479888759
N	33.20745402021115	-25.51561876294084	4.85131292185069
N	34.64458427566762	-25.66312291847043	7.30421933869768
N	34.78687817361646	-27.68519205835251	3.79849143816432
C	32.96466754711051	-26.53297145650193	2.63765113205164
C	32.91553643677651	-24.01750738014277	6.76424066076543
C	36.40740814975261	-26.87848217992856	8.49371282701462
C	36.68176520344776	-29.16152210554043	4.24560970007307
C	30.78270781618690	-22.65052035193656	4.98005503969718
C	33.50935393558409	-22.91814742945618	9.60088413159413
C	38.78101648940967	-28.83609320482336	8.80882679390985
C	36.22119932874826	-30.13551707769553	1.34182844522073
C	32.62700253779627	-25.60497645708951	3.61833393812049
C	33.86656208226385	-24.58253193278087	7.61044738314239
C	36.79517549880945	-27.75339929457517	7.48484046396874
C	35.67440195295296	-28.65422131510280	3.43285141163249
C	31.61984640775078	-24.56575630562400	3.45054241648697
C	34.16678651203731	-24.10009982210769	8.95122031004829
C	37.91535024472704	-28.67879579911338	7.59337280732999
C	35.42803315440551	-29.08661542786419	2.06330396027526
C	31.61427589601335	-23.84415182264932	4.61317257089966
C	35.14415721376710	-24.92125920211890	9.44457552268809
C	38.01093081410569	-29.30916737887060	6.38218723674520
C	34.36631798439457	-28.35268106904825	1.61605856438049
C	32.61535891588933	-24.45420350956595	5.47704605047568
C	35.43232603695441	-25.89082556931969	8.39672562946122
C	36.93763165823962	-28.77181427532686	5.55728312966723
C	33.98332549575902	-27.47532366268817	2.71550872524462
N	36.22368224414004	-27.83718020712101	6.24729275084800
Fe	34.63790503497895	-26.75276338346721	5.59103935548079
C	34.10464875069129	-31.32767800435330	7.35251512753846
C	35.36221248706520	-31.92152269500042	6.73775340501328
C	32.19063665520201	-27.54190377339919	6.89650647923754
C	33.49715969336775	-27.85722300650567	6.19838522984911
C	33.59990207114716	-29.35066623528689	6.11016091547623
O	33.22781804054769	-30.03180143903442	5.18138318387989

O	34.08368620616900	-29.89020367838048	7.26885072863865
H	30.06643273611177	-22.40036031308676	4.18958612192432
H	31.40183063240263	-21.75926578607504	5.15440977737580
H	30.20686067594383	-22.82216742985129	5.90026883832089
H	31.42775826569697	-24.10647216318999	1.34555495331328
H	30.23498987094742	-25.26281279883250	1.94036307235156
H	30.07628500197531	-23.54731624395608	2.33855956887168
H	33.74353210620644	-27.40940693051213	-0.22784706198878
H	34.16301018993294	-29.11891820427977	-0.38986624369706
H	32.63138487761923	-28.64883670796454	0.35864613522280
H	35.87830321777848	-30.25893576377203	0.30864527117866
H	37.28985368599496	-29.88294722473609	1.30387198033448
H	36.14185473152302	-31.11607430511825	1.83210731599699
H	33.91543984625833	-22.73222192056956	10.60133904978428
H	32.42445519167958	-23.05985209506385	9.70876042141872
H	33.65236224423126	-22.00075855324684	9.01300382635201
H	36.92079742598831	-24.73718169662750	10.66236986849081
H	35.68868557305094	-25.79596261031526	11.34911450807361
H	39.56185190175450	-29.58823934538534	8.65125029257851
H	39.28146453490528	-27.89504044703767	9.07607850678850
H	38.19949516302758	-29.14819496039995	9.68784563270650
H	38.52879383801442	-31.27323901518660	5.63053137826193
H	39.57342263207753	-29.97490695391851	5.04764123923969
H	39.73833639660668	-30.56319796476894	6.70680698341738
H	35.46591842871970	-24.04234600880354	11.38966844324133
H	36.25424939282617	-31.48532441285347	7.19222930131821
H	35.37991288180932	-33.00693913688225	6.89230245153604
H	35.39379891345004	-31.72062974340484	5.66634454021780
H	33.20975580935954	-31.72494292117897	6.86758389674351
H	34.05401157198938	-31.53663773063195	8.42409458946292
H	32.02980944445033	-26.47838209584036	7.04584228247150
H	31.35342286168236	-27.94172992421613	6.30535975136145
H	32.15562698499409	-28.04637588458908	7.87235968589583
H	32.41265311168805	-26.48320337879503	1.70373420165596
H	36.95706851623153	-26.93340408437304	9.42881018143593
H	37.32784283317537	-29.92246879117284	3.81836278014778
H	32.36780160065482	-23.15744396983635	7.13783012369256
S	36.42300922049618	-25.17973978264083	4.65730936917578
C	35.96533114165368	-23.43477425967165	5.00079341691461
H	35.00789198106976	-23.16542101932901	4.53834370318326
H	35.88645427919569	-23.23908476491911	6.07726661711649
H	36.73658929920207	-22.77017297617471	4.59162773666687

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B3LYP Scan/Thiolate IPC Model/RKS/1.9 Angstrom Fe-C Bond Length Constrained Optimization

C	30.81804167529857	-24.34309920569859	2.20302679121243
C	35.84796283548249	-24.84800692591860	10.77059865955230
C	39.00547796649539	-30.33931162838778	5.93535964883647
C	33.69894265933074	-28.38484713327580	0.27819729509531
N	33.23753192853068	-25.48334976121708	4.84007751858187
N	34.67066847355611	-25.62909005169856	7.29159069247778
N	34.81270907698431	-27.66324929424229	3.79038459259444
C	33.00239953716721	-26.49814806795186	2.62373462692667
C	32.91836588114010	-24.00464396125976	6.76402667621725
C	36.44135064286336	-26.83725777974015	8.47742323877429
C	36.68885767704680	-29.15923195998282	4.24835827540163
C	30.76709394622526	-22.65721391454870	4.98528164716370
C	33.49177957295583	-22.92209910654098	9.61282527326773
C	38.79461028436666	-28.81784028474328	8.80823448861617
C	36.20066036874444	-30.16341226177665	1.35634985499803
C	32.66029976521722	-25.57223965377040	3.60519459428733
C	33.87620458123481	-24.56304115433760	7.60731969253855
C	36.82228070246279	-27.72171970004158	7.47389164921419
C	35.68529248090985	-28.64836726449641	3.43218741015057
C	31.63957972480326	-24.54527466529740	3.44188151410942
C	34.16886124541877	-24.08692838079267	8.95232756537219
C	37.93224733028843	-28.65924745056876	7.59061031182106
C	35.42858764113098	-29.09186418705550	2.06739966671323

C	31.61927337197119	-23.83381220880597	4.61063932768805
C	35.15918153603741	-24.89676824668798	9.43865844104973
C	38.01942011882133	-29.30211783921101	6.38557230911797
C	34.37749503644482	-28.34598429019559	1.61493719307948
C	32.62685366491682	-24.43633347383527	5.47268993085636
C	35.46083789878352	-25.85423843118805	8.38309567885514
C	36.95142386341243	-28.75944672703929	5.55615032709844
C	34.01072001828231	-27.45151692503574	2.70668423692037
N	36.24869712019562	-27.81030055773503	6.23768703637541
Fe	34.69218967194467	-26.69819950012418	5.56572126031154
C	34.10437306780329	-31.38912225848823	7.32424325711024
C	35.37992047266343	-31.93238332576067	6.70071880147572
C	32.12796432978035	-27.56319600351280	6.93352598170653
C	33.40989689602259	-27.92469414222098	6.24501215675059
C	33.52190174226723	-29.39789687474026	6.13823457433961
O	33.14628685989744	-30.06363805158242	5.19764466423014
O	34.04618361300765	-29.95082194043222	7.27277661806692
H	30.04906048499345	-22.41175427460725	4.19484092768862
H	31.37050673357228	-21.75709098141377	5.16959079249238
H	30.19130338247238	-22.84608425788503	5.90220820310181
H	31.44224403539303	-24.07199285523311	1.33983410215415
H	30.26872699890069	-25.25303216545226	1.92381916742203
H	30.08051062820236	-23.54379516633289	2.33565282751355
H	33.75733709325637	-27.41578914829985	-0.23700467601698
H	34.15289762386512	-29.13276287472248	-0.38113551600087
H	32.63206862600819	-28.63268849360417	0.37021824756605
H	35.84968546733455	-30.29595693280913	0.32694590261668
H	37.27322985449023	-29.92917280262285	1.30862409022487
H	36.10856569604638	-31.13556301303618	1.86095345472522
H	33.89224416031182	-22.74037318480225	10.61637677365408
H	32.40888881643707	-23.08155780900247	9.71625467478590
H	33.62158863935333	-21.99605143517419	9.03535734660543
H	36.93109661785883	-24.69837778000685	10.66192231192405
H	35.71313546606944	-25.78096032291152	11.33612910321515
H	39.56703842691592	-29.58000704480319	8.65715700546488
H	39.30557786218493	-27.88078944185152	9.06998486490119
H	38.20844905278891	-29.11701662709735	9.68869393303994
H	38.51197524071377	-31.27982350053466	5.65216784736390
H	39.57399146021943	-30.00139558259308	5.05795405198965
H	39.73005169898489	-30.57584065529382	6.72273216269362
H	35.46484144985059	-24.03123710457839	11.39248559100302
H	36.25768761573968	-31.48174874600459	7.16845173941160
H	35.42801977058492	-33.02028589913967	6.82945050775891
H	35.40985660785704	-31.70489242400849	5.63447994007713
H	33.22226743953775	-31.79865815215951	6.82665662322401
H	34.05611933613068	-31.62421132616694	8.39057901729372
H	31.99299814241930	-26.49086354494308	7.04432063218353
H	31.27416936328487	-27.96846898983877	6.36761602910090
H	32.08602105219387	-28.03340532084586	7.92817855830459
H	32.45138628296471	-26.44789695307927	1.68911629060731
H	36.99222895351051	-26.89006094734349	9.41208055588123
H	37.32578591579771	-29.93135639539613	3.82715877300807
H	32.35698851096726	-23.15600818135530	7.14376634465712
S	36.41160699931546	-25.19885110637303	4.66598003112844
C	35.96554279234839	-23.45137796140917	5.00394979743727
H	35.01135343328497	-23.17708112181650	4.53982625420489
H	35.89230866290628	-23.25091471216277	6.07905294333306
H	36.74570501002410	-22.80213027334921	4.58801369930473

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B3LYP Scan/Thiolate IPC Model/RKS/2.0 Angstrom Fe-C Bond Length Constrained Optimization

C	30.82821091318948	-24.33240769021550	2.19891695640577
C	35.85312397898623	-24.84061034874450	10.76943139417214
C	39.00373736178990	-30.34289503827105	5.93832560702392
C	33.70151527034568	-28.38279604377297	0.27808930351416
N	33.25262878456256	-25.46883528591680	4.83383739454041
C	34.68453885867971	-25.61499470722720	7.28549841088314
N	34.82407699201615	-27.65187857371775	3.78599220587302

C	33.02061141432888	-26.48022229749501	2.61549505962111
C	32.92110644435870	-24.00057187701668	6.76394210713561
C	36.45901353434786	-26.81897573666148	8.46977106571541
C	36.69025521178184	-29.15852322077350	4.24945684932253
C	30.76249638978733	-22.65980678261463	4.98865863848044
C	33.48265995375811	-22.92798718183169	9.61905661961464
C	38.80376425380204	-28.80905622944417	8.80520002727808
C	36.18933725935879	-30.17659436099832	1.36374560947753
C	32.67678020227680	-25.55593636371365	3.59793201738472
C	33.88152965319250	-24.55643744342112	7.60597427451663
C	36.83644883901350	-27.70704528343798	7.46804627894313
C	35.68878318823496	-28.64557669752003	3.43179411374267
C	31.65035054606348	-24.53422421296989	3.43747936441872
C	34.16975276193328	-24.08394105099097	8.95325316529862
C	37.94158567149903	-28.65008064957797	7.58749857673672
C	35.42755685324974	-29.09410243444739	2.06933260864549
C	31.62363475496531	-23.82845800474950	4.60961779933777
C	35.16632962710844	-24.88801640721560	9.43641110543902
C	38.02365298191717	-29.29860146667160	6.38516738721131
C	34.38253461544190	-28.34169955470922	1.61355899390345
C	32.63374222463966	-24.42860331995078	5.47034269184958
C	35.47538853139016	-25.83889445474876	8.37696695696329
C	36.95723141960629	-28.75372093208817	5.55490885194583
C	34.02366648062159	-27.43892374043014	2.70117441799448
N	36.26037176492419	-27.79759171911241	6.23303570897992
Fe	34.71793456916782	-26.67255756929557	5.55361878571539
C	34.10803369244069	-31.41692990807670	7.32318705275382
C	35.38852739826613	-31.93609799820870	6.68984794729143
C	32.08631426255309	-27.57793296901615	6.94103062634756
C	33.36418226756982	-27.95998473525044	6.26768181035445
C	33.48152120447387	-29.42550240325806	6.15993489874893
O	33.10106802417803	-30.08745848660087	5.21732994768720
O	34.02996695492079	-29.97898630507341	7.28235458891918
H	30.04371859129449	-22.41574280256147	4.19842764220841
H	31.35901543106622	-21.75610379266649	5.17807628464057
H	30.18683693089698	-22.85698562707611	5.90394038324314
H	31.45051431012524	-24.05067866309579	1.33768428026579
H	30.28747966009494	-25.24569243540937	1.91397361459526
H	30.08322051674085	-23.54065643107057	2.33530939832280
H	33.76602415030497	-27.41700105959550	-0.24254690959104
H	34.14867523593301	-29.13769266817453	-0.37796508142369
H	32.63295650778143	-28.62204492271021	0.37327856525960
H	35.83476828610769	-30.31338077980218	0.33610458555501
H	37.26370180132530	-29.95139414791322	1.31180713711300
H	36.09081136166692	-31.14451811486126	1.87521279218994
H	33.87973003407195	-22.74883121420679	10.62443939063480
H	32.40079467159853	-23.09617537202336	9.71945472251013
H	33.60634784104023	-21.99758248094209	9.04720190416429
H	36.9352777218401	-24.68216174627816	10.66305772451525
H	35.72484542157681	-25.77743339843654	11.33008495086804
H	39.57242033567186	-29.57547001486765	8.65625273122148
H	39.31942960065385	-27.87371004318854	9.06395850215760
H	38.21655542221964	-29.10257992370954	9.68687997539555
H	38.50533528664055	-31.28210178544513	5.65941239537417
H	39.57324125144881	-30.01177656716270	5.05891489488598
H	39.72789666162796	-30.57986482206346	6.72597974526299
H	35.46294535026780	-24.03000528042721	11.39500374526677
H	36.26129096507398	-31.47550833844948	7.15715059213213
H	35.45371720098917	-33.02412347438467	6.80979497457614
H	35.41028678396982	-31.69959482810012	5.62533685711494
H	33.22945837221925	-31.83509522536774	6.82667619109637
H	34.06803472267607	-31.66051673399959	8.38797043876653
H	31.95684722247477	-26.50240618419528	7.02744622919826
H	31.23151022074794	-27.99332387708437	6.38298940443756
H	32.03764556847683	-28.02631499806051	7.94635803337260
H	32.47060060040747	-26.42891704313786	1.68029929027639
H	37.01084774066268	-26.87081657068038	9.40397154038720
H	37.32204648807955	-29.93648618731964	3.83114023022484

H	32.35329506860223	-23.15767754877941	7.14704589682698
S	36.41411441526845	-25.19899135018932	4.66777426259093
C	35.96859339691880	-23.45139035778609	5.00227632619598
H	35.01595817747766	-23.17713153154157	4.53574777868084
H	35.89496210171833	-23.24922479017400	6.07668751050129
H	36.75177009615336	-22.80671748182449	4.58520825479753

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B3LYP Scan/Thiolate IPC Model/RKS/2.1 Angstrom Fe-C Bond Length Constrained Optimization

C	30.83826149079954	-24.32068933608717	2.19478775499780
C	35.85634479180781	-24.83889237119397	10.76868472088178
C	39.00186970367206	-30.3468888302161	5.93727130124882
C	33.70487618684584	-28.37794734259383	0.27515676670945
N	33.26815423209590	-25.45492347033383	4.82648982912568
N	34.69876283128691	-25.60294996480201	7.27824197766159
N	34.83551137217265	-27.63910346116464	3.77929964197259
C	33.03870194569685	-26.46119810371199	2.60541151497214
C	32.92428923815075	-23.99832499009819	6.76356138805305
C	36.47681823542300	-26.80312997064072	8.46086982280474
C	36.69106714835752	-29.15732100966383	4.24803651743380
C	30.75859921312245	-22.66304221553350	4.99293256307888
C	33.47195165347693	-22.93905387129850	9.62626207886915
C	38.81453566888027	-28.80136167699331	8.79853003677925
C	36.17814224208428	-30.18759008559616	1.36850565749582
C	32.69335685116469	-25.53931394656311	3.58955248120401
C	33.88690834865638	-24.55240701945731	7.60417504414812
C	36.85125703395433	-27.69357108308644	7.46014687351455
C	35.69209863732020	-28.64157761116778	3.42900389939111
C	31.66134109286915	-24.52279075673772	3.43272302153405
C	34.16977656662418	-24.08501347415016	8.95433447427678
C	37.95165211841199	-28.64191798643461	7.58139336217109
C	35.42655335496558	-29.09456402521047	2.06877878061146
C	31.62859182636921	-23.82339304778625	4.60859079294310
C	35.17246281905098	-24.88351106300116	9.43407771936359
C	38.02798244734122	-29.29568108233958	6.38152318046917
C	34.38791267800101	-28.33535520682209	1.60959668067779
C	32.64126551315567	-24.42165025302656	5.46743149285048
C	35.489754440648642	-25.82645459249977	8.36999180666349
C	36.96296435189923	-28.74815571393117	5.55110323583348
C	34.03683427109819	-27.42477569371496	2.69321251250560
N	36.27231536292859	-27.78511091505229	6.22641949780914
Fe	34.74389476552373	-26.64768392077054	5.53981830074601
C	34.11370978683957	-31.43917795460775	7.33873029025138
C	35.39681793216359	-31.93596252125759	6.69312361075594
C	32.04010956711584	-27.59278855075451	6.93836783432340
C	33.31851395362286	-27.99608938191493	6.28821141263062
C	33.44139608798367	-29.45535168854971	6.18880960894117
O	33.05466180102314	-30.11945809226333	5.24894814320427
O	34.01411680207501	-30.00221066453344	7.30189914480469
H	30.03899904940513	-22.41981572896425	4.20316397696895
H	31.34827692576788	-21.75601538345544	5.18801000583989
H	30.18324136834870	-22.86915676229692	5.90646421739217
H	31.45827214787596	-24.02728819333329	1.33569817956957
H	30.30656019132539	-25.23726077605071	1.90343198561695
H	30.08548439577298	-23.53708012758700	2.33575952617339
H	33.77590860151695	-27.41529155079294	-0.25045974169047
H	34.14526005421631	-29.13959219357206	-0.37771017282642
H	32.63460668837348	-28.60834826119395	0.37294362170512
H	35.81956097306064	-30.32878867232004	0.34283138877984
H	37.25408292602261	-29.97096238438974	1.31195979910199
H	36.07388221198142	-31.15116234237463	1.88696648739872
H	33.86435165473546	-22.76412894138821	10.63424183895833
H	32.39105169539418	-23.11602649775827	9.72191632673443
H	33.59028160760879	-22.00349111022708	9.06165447834581
H	36.93744364872646	-24.67106160959313	10.66558174738508
H	35.73463601797165	-25.78026253429694	11.32316951402562
H	39.57998235612734	-29.57121656388475	8.65070075133226
H	39.33421526069701	-27.86744309556620	9.05449232095611

H	38.22719467430471	-29.09031260620209	9.68164346129669
H	38.49853580840558	-31.28499940961770	5.66357098217322
H	39.57120019582846	-30.02271796926142	5.05513664786916
H	39.72658744889581	-30.58380569071415	6.72444885851018
H	35.45841506179598	-24.03548141968013	11.39864708890253
H	36.26576052484304	-31.46193906840691	7.15407595368775
H	35.48091383479721	-33.02306703237259	6.80939179609474
H	35.40555376564540	-31.69623140418133	5.62905073151713
H	33.23731286904685	-31.86938312588140	6.84880611112098
H	34.08638064518196	-31.68567573724966	8.40326034443299
H	31.91349619717839	-26.51469148354844	6.99601478669534
H	31.18853215783493	-28.02211277989107	6.38507771604435
H	31.98065082689644	-28.01558953063343	7.95515727198594
H	32.48958297763343	-26.40829653219312	1.66975452894667
H	37.02939886847317	-26.85459626390259	9.39468628281526
H	37.31709604304142	-29.94142107130206	3.83239974815286
H	32.34994048716759	-23.16160014637298	7.15057840564571
S	36.42235226284883	-25.19420699802199	4.66759123654645
C	35.97487232513496	-23.44715837346226	4.99967419548980
H	35.02378130194064	-23.17365608844270	4.53022751420338
H	35.89931327623351	-23.24442656088247	6.07356186463450
H	36.76038302642366	-22.80513513036615	4.58313785375755

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B3LYP Scan/Thiolate IPC Model/RKS/2.2 Angstrom Fe-C Bond Length Constrained Optimization

C	30.85322907071300	-24.30086688410206	2.18837788795222
C	35.85415882030146	-24.85317854050984	10.76986706778211
C	39.00177872694563	-30.35046328716878	5.92464277391562
C	33.71568631779643	-28.35990459602174	0.26187396835994
N	33.28508093912091	-25.44209521367209	4.81636017055866
N	34.70979884739022	-25.59965889800737	7.27065211664298
N	34.84695353882866	-27.62477701932997	3.76744273576690
C	33.06000534164978	-26.43645552892984	2.58958485228619
C	32.92652421864868	-24.00254862958920	6.76414591746262
C	36.49143206294081	-26.79738284728690	8.44987396428711
C	36.68954947835606	-29.15788068902579	4.24011688200808
C	30.75779256601915	-22.66615764260853	4.99918486071016
C	33.45644463395709	-22.96416203624042	9.63750492608312
C	38.82834581737890	-28.79726559885775	8.78266672874515
C	36.16937854029153	-30.19153607101904	1.36365539430783
C	32.71242717380156	-25.51953563915095	3.57754255511964
C	33.88944151177434	-24.55755342791968	7.60337377933640
C	36.86379324077364	-27.68713357018239	7.44790571911514
C	35.69486715087550	-28.63624417756789	3.41977574866206
C	31.67581599362139	-24.50728230131455	3.42597885445604
C	34.16556361572892	-24.09848828997001	8.95775248350932
C	37.96189213505086	-28.63825368905531	7.56798510000590
C	35.42730966905346	-29.08956119117885	2.06009080504331
C	31.63636717182151	-23.81750138012598	4.60740378621602
C	35.17390225918660	-24.89226781791954	9.43326392787107
C	38.03197433390530	-29.29563832073856	6.36964255685772
C	34.39724929682220	-28.32089733702610	1.59721629255536
C	32.65010649502945	-24.41687516829574	5.46384759057694
C	35.50026037910312	-25.82478179404125	8.36285508693564
C	36.96625345637953	-28.74636589606719	5.54137579556881
C	34.05263532168616	-27.40532498826246	2.67870349780069
N	36.28069814271903	-27.77851241746599	6.21585454460612
Fe	34.76774389576890	-26.62690816860674	5.52310957427482
C	34.13599592830492	-31.44118443792070	7.40833946604483
C	35.40214619694166	-31.93258987849532	6.72677617931256
C	31.98090876407720	-27.60344433483539	6.90686296480747
C	33.26905800627116	-28.03476710004118	6.30533321409851
C	33.39785074501135	-29.48956944577959	6.24739886636510
O	32.98302550633647	-30.17539921304012	5.33347863852816
O	34.01672365594881	-30.00600368832020	7.34887206817767
H	30.03643691985616	-22.42310633798097	4.21094747587485
H	31.34057565625937	-21.75594974094424	5.20017450469520
H	30.18400333365035	-22.88243480983044	5.91131225102438

H	31.46980486535287	-23.98144370991596	1.33600711556227
H	30.34046533900472	-25.22273232072598	1.88055244045673
H	30.08479522152060	-23.53447729635274	2.33928039364238
H	33.79884553169390	-27.39995481450391	-0.26700593969577
H	34.14771359743785	-29.12900792120156	-0.38788772443907
H	32.64255125586324	-28.57696018422352	0.35892501602201
H	35.80335026093925	-30.33943828253992	0.34155819063961
H	37.24600667799166	-29.98038397914669	1.29824718306058
H	36.06429109737613	-31.15023999520294	1.89081273197750
H	33.83941802905495	-22.79919679092986	10.65078288679157
H	32.37579238852356	-23.14792996349996	9.72198529830676
H	33.57427226292889	-22.02112539668606	9.08529332280093
H	36.93385309114859	-24.67376976161600	10.67104716604262
H	35.74045912340671	-25.80078559906396	11.31534625172381
H	39.59519889251264	-29.56520307670262	8.63192100934940
H	39.34656924568212	-27.86241392522019	9.03818651212508
H	38.24424814166081	-29.08854498776441	9.66721201388714
H	38.49586056449902	-31.28871373574159	5.65621182698221
H	39.56779408852449	-30.03029045288872	5.03888771246283
H	39.72965583466589	-30.58605281106809	6.70930446259787
H	35.44694893967758	-24.05953605342611	11.40624309963836
H	36.28060191958260	-31.44404590803174	7.15297921306065
H	35.50140755024072	-33.01733878753337	6.85311352879637
H	35.37301103294447	-31.70576276721308	5.66019107044641
H	33.24864528665391	-31.89129623906972	6.95751079466410
H	34.14895571240136	-31.66806691004621	8.47739364977659
H	31.84052361014963	-26.52554101973584	6.88632028883143
H	31.14048186874558	-28.08777130731692	6.38251048847550
H	31.91824823111392	-27.95152259702091	7.95229068425007
H	32.51323022320502	-26.37920883404334	1.65280179021856
H	37.04488001982043	-26.85011648059796	9.38313466999236
H	37.30971537276114	-29.94747270091784	3.82597321670512
H	32.34565984731457	-23.17267900227601	7.15619312023571
S	36.43963539857072	-25.18880237420950	4.67594749117435
C	35.97779451771947	-23.44188386409440	4.98686346685255
H	35.03245513109253	-23.17743926068892	4.50137647252979
H	35.88626028929949	-23.23168070442139	6.05784369453242
H	36.76690134781904	-22.80054223991385	4.57623622121429

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B3LYP Scan/Thiolate IPC Model/RKS/2.3 Angstrom Fe-C Bond Length Constrained Optimization

C	30.85322071914637	-24.31292603677702	2.18284945276050
C	35.84645048189294	-24.85476948419872	10.76919081480908
C	39.00635056916427	-30.34865903236931	5.92778191175549
C	33.73910938377341	-28.35325085266472	0.25179112934555
N	33.30414495664868	-25.43279093684757	4.80304433218730
N	34.72278041180887	-25.59000332474368	7.26010971389186
N	34.86364947734479	-27.61238214522704	3.75944496373776
C	33.08141683225822	-26.42491425834042	2.57501869558024
C	32.93098703560096	-24.00199614594384	6.75558069635796
C	36.50219119883130	-26.78607381407121	8.44472401241319
C	36.69956197852439	-29.15217972430211	4.23900187837013
C	30.74435958269900	-22.68579265234496	4.99778808065258
C	33.44243721780222	-22.97417437311584	9.63586880510669
C	38.83031716561644	-28.79466507405844	8.78467053399877
C	36.18539903006501	-30.18860659210554	1.36329427801910
C	32.72925917939134	-25.51224479987037	3.56495159192914
C	33.89519753036735	-24.55363918675468	7.59509998232387
C	36.87425583698524	-27.67703579419000	7.44401054780443
C	35.70914265464313	-28.62819445171991	3.41539655279540
C	31.68183323534781	-24.51103649769476	3.41784153205925
C	34.16222553479530	-24.09979846145918	8.95285042695693
C	37.96731058568746	-28.63315843200979	7.56789520406175
C	35.44398994002288	-29.08374715746836	2.05612891592213
C	31.63642805053036	-23.82512006301363	4.60133165749882
C	35.17298541429702	-24.89027782429170	9.42905322403098
C	38.03706385877020	-29.29215644004688	6.37051250155979
C	34.41761301224680	-28.31278927203213	1.58868215946794

C	32.65793299749161	-24.41574596489746	5.45453581014376
C	35.50928774740150	-25.81559437743525	8.35582288937626
C	36.97541861043894	-28.73889240932890	5.53962167914910
C	34.07319885374654	-27.39390883651162	2.66714322798372
N	36.29272112072944	-27.76603234812880	6.21061045729430
Fe	34.79447365478200	-26.60281109221079	5.50667500365947
C	34.13398149036620	-31.46579586194153	7.40985430894583
C	35.36120665044550	-31.95567734636873	6.65962163391495
C	31.97116796269790	-27.57757780969596	6.97270998159641
C	33.22360480049512	-28.06012282116831	6.34250606974362
C	33.32975630465985	-29.51121516688710	6.30221650778899
O	32.84687479343414	-30.19270404358009	5.41677114089333
O	34.01544636273571	-30.02988853015866	7.36068622384432
H	30.01701813710884	-22.45175755870448	4.21231756150273
H	31.31553815276667	-21.76795463095733	5.19770311396624
H	30.17674462046937	-22.91045126992697	5.91178831681757
H	31.46251393544564	-23.98134742492494	1.32984504662679
H	30.35418633312706	-25.24170385857905	1.87337149241647
H	30.07342363206976	-23.55901444533133	2.33819451906374
H	33.82607127233639	-27.39489458862047	-0.27935082274994
H	34.17056799103499	-29.12524393523369	-0.39493744838328
H	32.66517588338141	-28.56719089865926	0.34680624712706
H	35.82237612769378	-30.33649178960532	0.34012206010205
H	37.26274601073163	-29.98007869836179	1.30128192725513
H	36.07660704880309	-31.14685225934806	1.89059526674629
H	33.81716807578767	-22.81510325142641	10.65315932017107
H	32.36215636578927	-23.16427829843393	9.71109207171582
H	33.55894609645073	-22.02618925892692	9.09190982291317
H	36.92446863494685	-24.66170489558375	10.67734711304920
H	35.74157896078333	-25.80841932269072	11.30581583912288
H	39.59585714492896	-29.56421518895597	8.63547109386667
H	39.34998850232334	-27.86111308333869	9.04195897060636
H	38.24339577667555	-29.08512351127450	9.66763560956469
H	38.50065319532239	-31.28662784353009	5.65791729211431
H	39.57510234836456	-30.02922634639264	5.04348259776078
H	39.73200877550821	-30.58488031158828	6.71434444110880
H	35.42677792863016	-24.07161457158487	11.41042171337407
H	36.26239323191316	-31.47397725137437	7.04397083899176
H	35.46284537251807	-33.04173011310789	6.77126791800494
H	35.27748081124556	-31.72005470812699	5.59768237220019
H	33.22318323641151	-31.91235538107151	7.00492590674241
H	34.20275149092622	-31.69614964897557	8.47594213163553
H	31.78229346044260	-26.52198530952956	6.78854041618586
H	31.10034349573368	-28.17589937393029	6.66095488822358
H	32.05756102783655	-27.71830440972967	8.06510075022862
H	32.53500415520243	-26.36876141975510	1.63798738483094
H	37.05267919832319	-26.83992437600122	9.37967345051703
H	37.31768823819325	-29.94490641804807	3.82774446194869
H	32.34309129586891	-23.17784988966301	7.14941372570330
S	36.46108466240883	-25.17821821108103	4.67855189576248
C	35.98897348365051	-23.43277431483839	4.97986120472754
H	35.04601651353322	-23.17469888603796	4.48663759820483
H	35.88941094464151	-23.21929127872023	6.04928956013225
H	36.77886289198049	-22.79057243205196	4.57218820636998

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B3LYP Scan/Thiolate IPC Model/RKS/2.5 Angstrom Fe-C Bond Length Constrained Optimization

C	30.99627767439486	-24.07833679759780	2.12792861771114
C	35.72903814235409	-25.30901761441483	10.79017054392743
C	38.98975163824156	-30.45845747340710	5.63119900857070
C	33.89548625097751	-28.03096025934375	-0.00861481944543
N	33.34871401025935	-25.45665415974482	4.71948205505991
N	34.68991405532335	-25.81131398126301	7.21236660658416
N	34.91916106706915	-27.53379955549549	3.57607134437058
C	33.20707187912145	-26.23474031159014	2.40568703113340
C	32.87216471334494	-24.23306958421641	6.78991152281770
C	36.52025983932511	-26.99674981469126	8.31856430485384
C	36.70226201031413	-29.15408500964892	4.00415202036816

C	30.76541335009014	-22.74740124288539	5.08766521739557
C	33.25531670031381	-23.45587177137686	9.76828637319459
C	38.88337519206112	-28.98071064990661	8.53414984420626
C	36.23182323236235	-30.02140695925560	1.07732523209290
C	32.82051726072264	-25.40949639749137	3.45687089247957
C	33.82106459995209	-24.83534910931109	7.61312542303815
C	36.90822559529158	-27.81627387826405	7.26442853042692
C	35.74439054302309	-28.55941173133555	3.19535358422484
C	31.77671670312600	-24.39993688486360	3.36836693520824
C	34.04142782161394	-24.48490303735939	9.01028544905163
C	38.00084301156527	-28.77535619918081	7.33777790890063
C	35.50540528495711	-28.93051184235184	1.80707744740064
C	31.67787497928103	-23.84048467940213	4.61458221459144
C	35.08310208524388	-25.26148914969734	9.43753417145522
C	38.04506662066117	-29.39987838161116	6.11967156674040
C	34.52538734949932	-28.09520343837142	1.35093350290253
C	32.66598729222401	-24.51182030817944	5.44260688898489
C	35.47934155762270	-26.07872188752237	8.29924295295059
C	36.98200883460656	-28.80669528760996	5.32243259824751
C	34.17422429185905	-27.22921177471595	2.46875926457847
N	36.31159598563317	-27.85316427524075	6.03352229793508
Fe	34.83759030197908	-26.65125168238369	5.36208294178410
C	34.46007894665099	-30.71978440967363	8.59005200390977
C	35.32197213476510	-31.65694859170728	7.75750001120808
C	31.74409031651319	-27.55347532871048	6.48608861063203
C	33.08452624563899	-28.15288646461068	6.32221802388210
C	33.27025667924310	-29.41246723058532	7.00422348073720
O	32.60521909892687	-30.39552237969062	6.68959808830364
O	34.24890616547696	-29.45311568032641	7.94081737960058
H	30.06092846455509	-22.44419570179293	4.30522429393091
H	31.32432075400343	-21.84989321802473	5.38912251401123
H	30.17201281242262	-23.05838008633865	5.95879727459084
H	31.63941605970937	-23.67722234098104	1.33152673442039
H	30.49980145699757	-24.96809865960273	1.71629056338792
H	30.21844133067225	-23.33238465372536	2.32494991778067
H	34.06112249271629	-27.05673116567884	-0.49026504313028
H	34.30127467373021	-28.79840694263547	-0.67700472088195
H	32.80749814400608	-28.17932150319774	0.03923216152557
H	35.88175400475624	-30.11626510779240	0.04346888364673
H	37.31450204507615	-29.83567233071347	1.04013655306292
H	36.09373530412698	-30.99821720673882	1.56170727962414
H	33.57431894961351	-23.39600622974785	10.81474036167903
H	32.17923240859587	-23.67998141450126	9.76723225113052
H	33.36931298652160	-22.45227982566582	9.33417323349641
H	36.79716919699050	-25.05533838524213	10.73970357162967
H	35.66134765815760	-26.30962908686006	11.24013662016647
H	39.65851869583391	-29.72962283789339	8.33740261416276
H	39.39207362650355	-28.05195446594402	8.82732224654601
H	38.31557149414448	-29.32238072425951	9.41143271426262
H	38.46108627100759	-31.37618014425952	5.33699158796996
H	39.5555900236183	-30.12132686061985	4.75147906547508
H	39.71797780824020	-30.73502221128313	6.40172586982414
H	35.25857858422567	-24.60566076010459	11.48618574129276
H	36.27203379213410	-31.18107226176600	7.50670392769350
H	35.52524702180919	-32.57762893877621	8.31763778666764
H	34.80826640978496	-31.92112052940397	6.83228474538047
H	33.49160824030695	-31.17575336614889	8.81219329422162
H	34.95534187487937	-30.45772291179593	9.52763643731219
H	31.41043710310526	-27.04156314825718	5.57975105037512
H	30.98394633300943	-28.26844875118578	6.82890809617401
H	31.82257311519116	-26.75574548222296	7.24621847742611
H	32.69931892638163	-26.09745741057139	1.45535143370090
H	37.07952481978429	-27.08829888473942	9.24535065020362
H	37.30132769278030	-29.94464302262099	3.56169099568016
H	32.25250830609903	-23.46006227996456	7.23569700983208
S	36.53361008554750	-25.15168471607272	4.84470538920457
C	35.82456907188666	-23.47159242438280	4.65233532104961
H	35.08657383094864	-23.42674676435546	3.84440256786101

H	35.34778852412207	-23.12658791488558	5.57630170294739
H	36.64540785062424	-22.78504421420816	4.41233615864933

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B3LYP Scan/Hydroxide IPC Model/RKS/1.7 Angstrom Fe-C Bond Length Constrained Optimization

C	30.66791332626758	-24.41643645469046	2.21333270472979
C	35.49268992347111	-24.82768452866937	10.91009313515964
C	39.01808852014392	-30.09793913076221	6.08846432503966
C	33.80428067574207	-28.27793609881336	0.30005404015889
N	33.04686090539993	-25.50343343795241	4.90781506270018
N	34.42759427633256	-25.61947130663722	7.39908177492554
N	34.73363522869241	-27.62080248715365	3.87686007305183
C	32.90494852748039	-26.51517259222447	2.68279711810773
C	32.68441680777622	-24.00700756740612	6.80966288323685
C	36.19023314645725	-26.79786173521391	8.62523409469419
C	36.69456566643288	-28.99443484806642	4.35460804753402
C	30.54532737229339	-22.70422875490553	4.97635415935463
C	33.16679372287448	-22.91402934325091	9.67720602227512
C	38.63093558078417	-28.67198341981951	8.99201105588897
C	36.38677756721430	-29.91321040954272	1.40713222617455
C	32.50302556496524	-25.60788392278422	3.66060565097422
C	33.62102256346685	-24.55600890999169	7.68478686832048
C	36.64070499737847	-27.64956912043410	7.62018211453521
C	35.68747435166988	-28.52249020924754	3.51858713856357
C	31.47051751878490	-24.59645208061974	3.46823365685660
C	33.87107293165661	-24.07425939091664	9.03731887235310
C	37.79978430442178	-28.52674197498320	7.75102078418832
C	35.51255862957130	-28.93036673024065	2.12799963989289
C	31.42052039349507	-23.87232921797263	4.62893309450237
C	34.84835126607096	-24.88037997724311	9.55619992678977
C	37.96302436316158	-29.12811196419768	6.53261327606326
C	34.42633137310991	-28.24428460772311	1.66405969311444
C	32.41725776547343	-24.45606208385705	5.51731801749303
C	35.18895049498384	-25.83672989537716	8.51027612416799
C	36.89026294025949	-28.62248541004764	5.68251691811664
C	33.96052412529487	-27.41798556607806	2.77455154910952
N	36.11100293474195	-27.74312742868458	6.36834804485757
Fe	34.50602583822385	-26.70712298446307	5.67318550630489
C	34.05999538279665	-31.33179711887870	7.33234080001009
C	35.35648362159098	-31.86574049666637	6.74185613511749
C	32.05535233302376	-27.59154785154215	6.92634011395643
C	33.38547549965055	-27.85319894912819	6.23964541348874
C	33.51920319973791	-29.33928083192968	6.12477021589269
O	33.19731669792091	-30.02031263904890	5.17543221497054
O	33.99296660190775	-29.89687629725794	7.28728935516704
H	29.84044757623753	-22.47326561170030	4.16962455971540
H	31.13156701130567	-21.79406211562669	5.16795234255484
H	29.95301542685540	-22.89499390238799	5.88235108517222
H	31.30289400468495	-24.14786783806684	1.35698585741743
H	30.13333627352753	-25.33537591509228	1.93497416904420
H	29.91932108685753	-23.62399864568607	2.32455701198648
H	33.80457325306643	-27.28619955166587	-0.17406202422612
H	34.34141966823437	-28.95884932522002	-0.36955681258984
H	32.75809156328569	-28.61319032213388	0.33684577680022
H	36.10209431253399	-30.00791884817128	0.35318824900833
H	37.44382392252571	-29.61426103528953	1.43441758307683
H	36.32789305635671	-30.91645467154956	1.85273390364035
H	33.53011119171713	-22.73456743367018	10.69531365507827
H	32.08163528356892	-23.07840224551107	9.74138832955617
H	33.31217971917279	-21.98440446537938	9.10885482346825
H	36.57553573013170	-24.65336897380635	10.83926500709502
H	35.36016298934075	-25.76862747530995	11.46264299479673
H	39.44607863585652	-29.38985332304012	8.84753817193444
H	39.08426518719738	-27.71752131385670	9.29486453965087
H	38.03332103832729	-29.02382929269247	9.84487031800707
H	38.58446875463626	-31.05516551297498	5.76616259265920
H	39.59354761198216	-29.70702283774439	5.23774356786727
H	39.73058665000165	-30.31748452514726	6.89188099551469

H	35.07138056791259	-24.02548953707800	11.52628310323887
H	36.21876305224454	-31.41046956765896	7.23416443396948
H	35.41005482416075	-32.95398411536226	6.86799910523038
H	35.41177788477605	-31.63410319647779	5.67758742555305
H	33.19650422578680	-31.74714850356451	6.80686223982229
H	33.98360174280202	-31.57612503011800	8.39544979094549
H	31.85930674934403	-26.53455736728915	7.08621512612369
H	31.23318298288160	-28.00748473873387	6.32385340112518
H	32.02180308436475	-28.10497809559994	7.89835487931227
H	32.37881066592445	-26.47361139152458	1.73316525671840
H	36.71294998770060	-26.84574894593003	9.57652778757816
H	37.39310685600132	-29.71204770476877	3.93382091210094
H	32.10929483624107	-23.15827195023656	7.16878062173241
O	35.78986155429061	-25.41345716336087	5.01744280777752
H	35.44285902544219	-24.52873214415055	5.20352013170482

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B3LYP Scan/Hydroxide IPC Model/RKS/1.9 Angstrom Fe-C Bond Length Constrained Optimization

C	30.73652965059010	-24.34994122320697	2.18126698430248
C	35.54371544995922	-24.77094859044524	10.88548640908876
C	39.03909194175901	-30.08710281420365	6.08455069778959
C	33.84699752333755	-28.24130703909776	0.28296462559157
N	33.12209317868641	-25.42883986101184	4.87441088952738
N	34.49733001813637	-25.54616371091809	7.36402341171488
N	34.79909193689094	-27.55661177556266	3.84920882582379
C	32.98198263780092	-26.43923255939123	2.64807853484494
C	32.74343490792754	-23.94295895271476	6.78158647902542
C	36.26014134615413	-26.72342134436606	8.59218917418891
C	36.73924617932492	-28.95577257015574	4.33701235418887
C	30.59622816539003	-22.65063165856229	4.95134745034617
C	33.20585145722718	-22.86821233492140	9.65917230220441
C	38.67205173620817	-28.63140065263585	8.97564521793551
C	36.40572729891012	-29.90644204314347	1.40124499529398
C	32.57977368086862	-25.53215004880343	3.62563349662877
C	33.68133329117567	-24.49076085282226	7.65582385116320
C	36.70363429704352	-27.58364139752418	7.59126966910261
C	35.73752171187466	-28.47796176479366	3.49780402379671
C	31.54041635828660	-24.52748651082666	3.43571614513338
C	33.92311603971056	-24.01662115854495	9.01233690856476
C	37.84791644277013	-28.47884039557315	7.73088778068349
C	35.55201339155765	-28.89889585376475	2.11254503517278
C	31.48242302645806	-23.80913031549241	4.59961520208377
C	34.90606283081519	-24.81774786180354	9.52821039071912
C	38.00253704257323	-29.09271657240501	6.51766401288145
C	34.47627638068563	-28.19983815808233	1.64343729752688
C	32.48232383195226	-24.38859630901317	5.48690503761182
C	35.25732964696722	-25.76419993436664	8.47702727693053
C	36.94020188180115	-28.57521814954175	5.66176454575057
C	34.02689099298714	-27.35379603482790	2.74570145335155
N	36.17415648978633	-27.67669119853957	6.33879778423266
Fe	34.59579528149904	-26.61524903231772	5.63062427623663
C	34.08346492366086	-31.35228593695541	7.29570870306379
C	35.40073670672155	-31.83323470217380	6.70656125641470
C	32.02617075195717	-27.57176278574429	6.93753181376252
C	33.33276428188424	-27.88611408758387	6.26280676383978
C	33.47743744635463	-29.35194640568971	6.13107236820974
O	33.16437442375554	-30.01917419516451	5.16735766044231
O	33.97602308747513	-29.91876673413044	7.27855242982055
H	29.89147377701607	-22.42101958906937	4.14410203186279
H	31.17399478181126	-21.73646609440939	5.14976557927933
H	30.00319149426189	-22.85147583094201	5.85472017717125
H	31.36959714566842	-24.07589034556182	1.32519684561280
H	30.20749839049273	-25.27157844987203	1.90119848133052
H	29.98315437778381	-23.56225623019709	2.29413319199212
H	33.85585503090055	-27.25479317195154	-0.20193999749245
H	34.37275528874721	-28.93557172185549	-0.38194758288555
H	32.79720000314796	-28.56395923954573	0.32889983532777
H	36.11740998955845	-30.00707818545182	0.34882097749010

H	37.46854185591926	-29.62806395678729	1.42352367872859
H	36.32820437693635	-30.90345487181549	1.85783280260714
H	33.56219450335799	-22.69507023328016	10.68085283429368
H	32.12178485132914	-23.04213854574678	9.71600604205773
H	33.34628168592279	-21.93200162942090	9.10037074478919
H	36.62575296671004	-24.58888900596129	10.82134885449194
H	35.41494558332766	-25.71692791771620	11.43029905643957
H	39.47956287683038	-29.35882072024158	8.83598662000905
H	39.13515219528941	-27.68170999193526	9.27886286381293
H	38.06702398693037	-28.97483006494755	9.82677426444907
H	38.58756245300167	-31.04001492191039	5.77409840979994
H	39.62141737742247	-29.7178387798649	5.22878863323610
H	39.74797898453404	-30.31012320911385	6.89023745577378
H	35.11419313646982	-23.97628838429834	11.50577443904433
H	36.24379990505638	-31.35866737493923	7.21348936582537
H	35.48899119586972	-32.92128658375129	6.81332058457980
H	35.45707737721739	-31.58005470468082	5.64716742533073
H	33.23713641064268	-31.78141723411126	6.75393929652640
H	34.00503561441270	-31.62029856579957	8.35295084760471
H	31.86311479772097	-26.50419221901690	7.06389810691199
H	31.18658552679015	-27.98491343886743	6.35495927658516
H	31.97905525674553	-28.05549962446850	7.92602510987768
H	32.45664643417985	-26.39710797846797	1.69799753346492
H	36.78142080493733	-26.77193258664882	9.54427643971574
H	37.42671864553294	-29.68760940897637	3.92239743277399
H	32.16113215168041	-23.10043405200863	7.14382437969613
O	35.85682241052547	-25.34964362103534	4.98644355276883
H	35.50803172639352	-24.46679372638696	5.17867089012586

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B3LYP Scan/Hydroxide IPC Model/RKS/2.0 Angstrom Fe-C Bond Length Constrained Optimization

C	30.77303408864987	-24.31365866484433	2.16482367371700
C	35.57079666281671	-24.74286898631703	10.87311579694469
C	39.05056695410971	-30.07980625769046	6.08061403715885
C	33.87050506219527	-28.21989735540197	0.27302782575328
N	33.15954120705570	-25.39310708192540	4.85762038732771
N	34.53232980921702	-25.51222795125408	7.34743565499439
N	34.83082022959656	-27.52437690869770	3.83536595792992
C	33.02113719777289	-26.40003771798238	2.62949031751320
C	32.77220296098494	-23.91427473138573	6.76877301867275
C	36.29648578384107	-26.68700658035351	8.57624043137343
C	36.75918953221375	-28.93791052008928	4.32902853870112
C	30.62277097188688	-22.62428076018964	4.94037683596285
C	33.22459106060237	-22.84823861371440	9.65065643034102
C	38.69551982430162	-28.60965783564097	8.96566249299733
C	36.41412481868119	-29.90303568453939	1.39917109473405
C	32.61860341501195	-25.49394096710120	3.60761414112871
C	33.71086297021757	-24.46136829322197	7.64234188554769
C	36.73605914784638	-27.55105019916764	7.57698380204330
C	35.76081928336108	-28.45640812910011	3.48801638581909
C	31.57637716480295	-24.49212186400534	3.41949103421277
C	33.94863091312278	-23.99056739799627	9.00055803362736
C	37.87322914868427	-28.45461457751653	7.72000213279406
C	35.57085433041052	-28.88305524632890	2.10522530684446
C	31.51397294880350	-23.77809939646012	4.58585252573485
C	34.93534818125373	-24.78808869578429	9.51476432059781
C	38.02232259613930	-29.07494546955887	6.50935714973401
C	34.50173810601442	-28.17622974845463	1.63252791410045
C	32.51465937480396	-24.35678695171406	5.47240898845190
C	35.29220557895329	-25.72957121714067	8.46115989084791
C	36.96416882000925	-28.55225605510538	5.65163176586936
C	34.06030990854628	-27.32062305058954	2.73042532520177
N	36.20534748448432	-27.64407712839148	6.32472314343798
Fe	34.64034170352943	-26.57022793665173	5.60995432321399
C	34.09737944714089	-31.36075275755040	7.28641743404521
C	35.42112956587589	-31.81647535255365	6.69227072549780
C	32.00368961484681	-27.56440706130871	6.93271117670089
C	33.30512857823962	-27.90343887504751	6.27309421022889

C	33.45388072081499	-29.36177267733483	6.13919096241709
O	33.13977433434828	-30.02481673289212	5.17195614190852
O	33.96920523725399	-29.92855898223107	7.27880820780024
H	29.91814261291618	-22.39465999215140	4.13301953426866
H	31.19666129183567	-21.70849197884930	5.14261671780146
H	30.02937989892771	-22.83038919901362	5.84234133972162
H	31.40560268514845	-24.03333542185148	1.31038164378837
H	30.24869664383036	-25.23673573606587	1.88070917654849
H	30.01579049542595	-23.52999604800609	2.27986376381631
H	33.88583056682198	-27.23584424840265	-0.21673257680376
H	34.39026577997873	-28.92127366170575	-0.38912006638063
H	32.81840172781222	-28.53453422943514	0.32193352020204
H	36.12412835920158	-30.00676597569609	0.34750658534242
H	37.47968711395499	-29.63512525688031	1.41920464162646
H	36.32709495346566	-30.89664180637450	1.86142519960853
H	33.57778291663311	-22.67776558252701	10.67388524724857
H	32.14122018340557	-23.02741032583179	9.70427451705657
H	33.36185859199971	-21.90893229157125	9.09625058580817
H	36.65207501752286	-24.55541495535854	10.81132088452627
H	35.44577042249917	-25.69132262398541	11.41451041611355
H	39.49866000914022	-29.34232688843828	8.82820131232793
H	39.16428632381145	-27.66222035572690	9.26728678256402
H	38.08783228346815	-28.94754903889652	9.81714170812003
H	38.59150066984763	-31.03080224839035	5.77531866551459
H	39.63535748922475	-29.71976669951364	5.22258361045093
H	39.75822140112584	-30.30421171835207	6.88701144749423
H	35.13658207298012	-23.95241157015582	11.49550759149526
H	36.25675804387136	-31.32972652329015	7.19986560956832
H	35.52821413204042	-32.90335904324731	6.79342584334762
H	35.47111381704365	-31.55683168941615	5.63408997174802
H	33.25666961700343	-31.79879557114758	6.74314705867808
H	34.02452014168518	-31.63676867100930	8.34197928850614
H	31.85180162898316	-26.49265094185914	7.03769367968698
H	31.16146549734711	-27.98193862698800	6.35616212453037
H	31.94688931315502	-28.02913422647204	7.93068665505175
H	32.49693593978092	-26.35669532058603	1.67884158332171
H	36.81762973252728	-26.73544722881273	9.52840663324339
H	37.44048947046063	-29.67728002882199	3.91754296698816
H	32.18613440659735	-23.07519934568864	7.13299372699559
O	35.89372815688589	-25.31445133853470	4.97037920756248
H	35.54197297319837	-24.43220560171215	5.16052822058345

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B3LYP Scan/Hydroxide IPC Model/RKS/2.1 Angstrom Fe-C Bond Length Constrained Optimization

C	30.81045189335759	-24.27587890970788	2.14858335790088
C	35.59716258006185	-24.71730025814022	10.86172155088598
C	39.06216832644582	-30.07240773741555	6.07519568862752
C	33.89511711966154	-28.19655385905424	0.26209626684397
N	33.19793536927497	-25.35716655433224	4.84047300948578
N	34.56838370830197	-25.47891979379986	7.33096286434717
N	34.86337060136974	-27.49099376324597	3.82073893344938
C	33.06168838481065	-26.35919221405891	2.60993281416494
C	32.80094674047034	-23.88717120061461	6.75677035581705
C	36.33466493997209	-26.65035523220739	8.55978259689083
C	36.77852133375630	-28.92039241235760	4.32076066520395
C	30.64945272106938	-22.59860937496348	4.93077224252495
C	33.24101151826839	-22.83230836851753	9.64400566192568
C	38.72173517894034	-28.58647141681124	8.95373046641501
C	36.42129052836229	-29.90015160854260	1.39724468426215
C	32.65854064668383	-25.45470817464935	3.58909134749832
C	33.74029885688183	-24.43373351832369	7.62957556784818
C	36.77057180691999	-27.51743848915105	7.56168865419066
C	35.78395449686847	-28.43464891486424	3.47784027176385
C	31.61328094153723	-24.45589853893460	3.40335767382644
C	33.97330499102948	-23.96706871901043	8.98988168290221
C	37.90051123486030	-28.42930642206104	7.70764622428813
C	35.58950462098728	-28.86684766785290	2.09755682846416
C	31.54615029442986	-23.74707889259098	4.57269242453843

C	34.96445033125115	-24.76031813354028	9.50204077643769
C	38.04295267644572	-29.05663768293506	6.49977656712004
C	34.52800238659746	-28.15123984539674	1.62077698971243
C	32.54747026118969	-24.32541689990341	5.45826554414289
C	35.32806473220874	-25.69562892781937	8.44536855008792
C	36.98841776434990	-28.52910728642656	5.64084466786182
C	34.09506281980547	-27.28576504529996	2.71404719036068
N	36.23776230384549	-27.61060731423440	6.31001162333152
Fe	34.68604615559462	-26.52429472059375	5.58887789758961
C	34.11385760540894	-31.36529500318221	7.28700225770305
C	35.43872114232803	-31.80103661277800	6.68098518888322
C	31.97669436950807	-27.55677650673589	6.91734678269914
C	33.27846192990959	-27.92004435273645	6.28212360371935
C	33.43062943350792	-29.37246051695166	6.15240142921615
O	33.11065300721365	-30.03530998038161	5.18585325476601
O	33.96748636543530	-29.93445413241179	7.28370072978646
H	29.94489185987532	-22.36870632432095	4.12343437663126
H	31.21911224738857	-21.68115876154488	5.13746919280941
H	30.05577645688799	-22.81080070114634	5.83114731749564
H	31.44211261535033	-23.98650319654274	1.29644368415150
H	30.29270497213282	-25.20085477728847	1.85865271944308
H	30.04777249255150	-23.49799759100845	2.26698164317399
H	33.91694929085282	-27.21481453523365	-0.23206179023433
H	34.40900152104587	-28.90468957016645	-0.39743046676660
H	32.84075826018243	-28.50319901681956	0.31351723030663
H	36.12971731180423	-30.00688931408166	0.34631331165222
H	37.48973888773282	-29.6437772697423	1.41528730963286
H	36.32371975285255	-30.89003355848853	1.86531910519855
H	33.58979017784043	-22.66573314663737	10.66939329824927
H	32.15844229856688	-23.01751215564376	9.69293044230416
H	33.37505795679205	-21.88906741000909	9.09548737948626
H	36.67744197411648	-24.52313355791681	10.80283168917417
H	35.47682460694105	-25.66887361951842	11.39872167519620
H	39.52139974848671	-29.32319992934847	8.81764364478860
H	39.19494309604968	-27.64084449839853	9.25412923625542
H	38.11230021831385	-28.92020372181544	9.80563933519203
H	38.59555698638965	-31.02243213740968	5.77838598277657
H	39.64675593064339	-29.72308941894421	5.21259484103776
H	39.77088077583326	-30.29587439991620	6.88094071454401
H	35.15714992807200	-23.93221974427862	11.48684264692094
H	36.27124445389638	-31.30326269525503	7.18285776609569
H	35.56212393497417	-32.88650334479557	6.77859347809900
H	35.47637521882191	-31.53811166700537	5.62307308987434
H	33.27423723046211	-31.81294896907092	6.75000650291134
H	34.05329877846658	-31.64434790239908	8.34250062290118
H	31.83204540374829	-26.48158368617817	6.99673179568967
H	31.13712949730098	-27.98330918054931	6.34275898796743
H	31.90578134339491	-27.99899171442247	7.92543513857524
H	32.53906210949820	-26.31392901048215	1.65851033986416
H	36.85610853958698	-26.69856206495352	9.51179557922933
H	37.45270658888826	-29.66816540765470	3.91271027450813
H	32.21038929168388	-23.05236944557983	7.12361689958652
O	35.93366813077321	-25.27694527545846	4.95367442173177
H	35.57738914487869	-24.39454488420682	5.13513416006272

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B3LYP Scan/Hydroxide IPC Model/RKS/2.2 Angstrom Fe-C Bond Length Constrained Optimization

C	30.85866228691470	-24.22076241453271	2.12397160520147
C	35.61009504166113	-24.72091527834047	10.85242233855281
C	39.07692312972169	-30.06252169775476	6.04949484303805
C	33.93074749959145	-28.15144185023618	0.23199259988467
N	33.23741138223730	-25.32299752201744	4.81637060992648
N	34.59747844606262	-25.45937403892996	7.31154234716554
N	34.89036570494134	-27.46005751756112	3.79646964840177
C	33.10487366485973	-26.31023183870784	2.57888206246279
C	32.82734053237540	-23.86931870662140	6.74359318245535
C	36.36431887952163	-26.63179405501304	8.53796584296111
C	36.79093381165106	-28.90815604702594	4.30080133194101

C	30.68454148232155	-22.56763253581019	4.91925109899183
C	33.24670742493176	-22.83992319704329	9.64260446161148
C	38.74756413579977	-28.57269803357588	8.92722871451636
C	36.43129354450809	-29.88613927150736	1.37751357204416
C	32.70173599832226	-25.41007391952077	3.56188694516519
C	33.76361284229559	-24.42048489166298	7.61611847608277
C	36.79755103691733	-27.49800855723037	7.53810687555211
C	35.80206342740667	-28.41460164295811	3.45611417001392
C	31.65703395514780	-24.41069603195124	3.38014520140005
C	33.98880668504502	-23.96398129136738	8.98118648150240
C	37.92396316890135	-28.41411088795934	7.68289731302552
C	35.60805860672565	-28.84414819367943	2.07521451061708
C	31.58428633227190	-23.71191015209153	4.55531945064776
C	34.98302811609136	-24.75524869690859	9.48994759520002
C	38.06050004207203	-29.04448463757626	6.47587949610954
C	34.55746560020535	-28.11530214303076	1.59382913871853
C	32.58219170834514	-24.29632683009786	5.43992558675050
C	35.35525112877502	-25.67985503488696	8.42683353287967
C	37.00569715847326	-28.51432902732824	5.61920402787736
C	34.12964189502660	-27.24569028686788	2.68548327257839
N	36.26124737915254	-27.58958642874825	6.28762450282432
Fe	34.72658601344464	-26.48830501394913	5.56076283425619
C	34.18375135947873	-31.32631590093209	7.39365052164207
C	35.45874703343755	-31.78379154875370	6.70315306865799
C	31.92430205646149	-27.53879927503263	6.85930447605140
C	33.24427877512122	-27.93806966244808	6.29625430519831
C	33.40140411849284	-29.38909336701691	6.23582536293475
O	33.01264545913124	-30.09369421348422	5.32334316479318
O	34.02949282238223	-29.89630897655697	7.34254953275794
H	29.97874598954508	-22.33616670244750	4.11345004489796
H	31.25168529156431	-21.64940292002884	5.12952534638422
H	30.09226593780371	-22.78550982602785	5.81912124237793
H	31.48994074999470	-23.90539613810986	1.28068015695221
H	30.35775540865205	-25.14852663658969	1.81441290471354
H	30.08271814251572	-23.45766816235763	2.25207126260932
H	33.96731046216910	-27.16946858610966	-0.26088590431729
H	34.43893437773549	-28.86523255688090	-0.42585317921531
H	32.87228708656927	-28.44466040426840	0.27766023213056
H	36.13952036494074	-29.99246410051907	0.32660440468105
H	37.50190326588563	-29.63884229130279	1.39571200993589
H	36.32519491541969	-30.87416222597722	1.84757401694083
H	33.58407394807746	-22.68625174808160	10.67381798717817
H	32.16427481928590	-23.02873930296960	9.67751734458705
H	33.38378026759830	-21.88885928460555	9.10846558781480
H	36.68906417176532	-24.51766151678322	10.79982888776497
H	35.49517440756679	-25.67877354156916	11.37933899780493
H	39.55238325536592	-29.30282985925617	8.78592317159210
H	39.21411588882756	-27.62543935032281	9.23265899193400
H	38.14157270875437	-28.91591816332165	9.77792802293559
H	38.60933598009930	-31.01446882079014	5.76042779180383
H	39.65545130718517	-29.71717675673193	5.18128608036833
H	39.79126020942358	-30.28154440701473	6.85151989930113
H	35.16158831654640	-23.94560576504712	11.48366543167647
H	36.32713562425661	-31.27645523652771	7.12834618609901
H	35.58593332670734	-32.86676851533460	6.82164483118505
H	35.41751919787708	-31.55067391715574	5.63830287164005
H	33.30686563334638	-31.79728421549395	6.94327861534936
H	34.20740555101807	-31.56089638945048	8.46122686359682
H	31.76328324181603	-26.46312088355710	6.83830086355727
H	31.10759565457067	-28.03379286201727	6.30741689869420
H	31.83296545311262	-27.88780844507997	7.90286955316033
H	32.58679895859940	-26.25738400802383	1.62539969221550
H	36.88583352732493	-26.68273070740625	9.48978128549957
H	37.45870638202504	-29.66245938939744	3.89419096969526
H	32.23258481938324	-23.03933082898676	7.11453988015218
O	35.97911451738800	-25.24754464185141	4.94351217090859
H	35.60073638505625	-24.36710602788510	5.08607717100231

B3LYP Scan/Hydroxide IPC Model/RKS/2.3 Angstrom Fe-C Bond Length Constrained Optimization

C	30.89865367070410	-24.17730181092007	2.10352725923901
C	35.63229625334171	-24.70842398457595	10.83899813172246
C	39.09038965071655	-30.05345583213350	6.03229223947581
C	33.96292053803830	-28.11489168378304	0.20889268996289
N	33.27424906974912	-25.28996795706245	4.79508632355406
N	34.62756575898013	-25.43546043772849	7.29286030169836
N	34.92400870149650	-27.42259266266223	3.77343947296911
C	33.14689827015270	-26.26487220594942	2.55179722019623
C	32.85226699486553	-23.84966383832863	6.73061603702013
C	36.39720023513380	-26.60553015393648	8.51759578778942
C	36.81143376927392	-28.88714215351762	4.28253250629449
C	30.71066818056464	-22.54404232711996	4.90959419560683
C	33.26003213311160	-22.83450902829225	9.63590474000861
C	38.77139704436224	-28.55697098841068	8.90750478800033
C	36.44581068189768	-29.86995520177848	1.36270349129661
C	32.74162742487685	-25.36970748731774	3.53830334723948
C	33.78854289055176	-24.40158763030677	7.60202275608833
C	36.82848165757886	-27.47165927032685	7.51704986458348
C	35.82762363232050	-28.38691624412795	3.43616461151366
C	31.69444063203484	-24.37274686749174	3.36046738343723
C	34.00924295903157	-23.95098223203776	8.96966400264455
C	37.94888338896480	-28.39463490056210	7.66295148411112
C	35.63162318112490	-28.81824639445757	2.05643946897107
C	31.61561744951578	-23.68254809746306	4.54041622856025
C	35.00729303601776	-24.73911914889085	9.47552035308993
C	38.08024320577835	-29.02842646810846	6.45705274495790
C	34.58868291240399	-28.08072609719157	1.57124600974953
C	32.61276557233320	-24.26928336628878	5.42373651017303
C	35.38555686063355	-25.65652246703366	8.40835201900382
C	37.02907073387129	-28.49220534590598	5.60000975282952
C	34.16690584305001	-27.20498578840510	2.65994508775400
N	36.29112728897847	-27.56027047087749	6.26650628233671
Fe	34.76911404702632	-26.44560908227401	5.53423094802333
C	34.21079669887466	-31.31513689290411	7.44250035359218
C	35.47114030440523	-31.77072154624820	6.72495690734986
C	31.89656103134315	-27.52741944156074	6.83398028821740
C	33.21735630073378	-27.95815967140070	6.30509968879517
C	33.37334234802548	-29.40531205676330	6.28108097585804
O	32.95453301171214	-30.12754570432560	5.39400635433378
O	34.04323195970837	-29.88690191613333	7.37310949611912
H	30.00540878871175	-22.31055023417195	4.10391944497399
H	31.27385169502307	-21.62483882490383	5.12625873150878
H	30.11768001196295	-22.76948208725736	5.80711712379906
H	31.53076187875435	-23.85291936178494	1.26424361576725
H	30.40286404380971	-25.10507486019886	1.78584649171792
H	30.11886068053506	-23.41871857413534	2.23499970941515
H	34.01056337167385	-27.13513705305868	-0.28747867291016
H	34.46372075047386	-28.83659136145945	-0.44594593455018
H	32.90123051363616	-28.39611669590569	0.25470338140120
H	36.15089940010223	-29.97989251534694	0.31304679840308
H	37.51823656876056	-29.63020825381633	1.37720261116559
H	36.33396020926210	-30.85462938984108	1.83838387927597
H	33.59232072419699	-22.68691588919425	10.66965902568800
H	32.17820873625097	-23.02768737351212	9.66478370640088
H	33.39570535853785	-21.87904121787513	9.10927432627025
H	36.70998832078290	-24.49767775148203	10.78909920027656
H	35.52311020328344	-25.67002588774425	11.36031827737748
H	39.57151072773625	-29.29247953150553	8.76733039723793
H	39.24416892226483	-27.61245273212819	9.21188950143007
H	38.16310834181767	-28.89514931758164	9.75859115114209
H	38.61727730379826	-31.00183647122634	5.74050059065603
H	39.67413992475031	-29.71105599731746	5.16633041282400
H	39.80074561095441	-30.27863317513193	6.83613832647747
H	35.17785032002062	-23.93973262480614	11.47407435980631
H	36.34572849126167	-31.25184903127288	7.12217467822980
H	35.61003884479740	-32.85121125247426	6.85220899173461

H	35.40068404604630	-31.55002904275575	5.65897215354807
H	33.32643103254581	-31.79988461313670	7.02282782667135
H	34.26445969446443	-31.53235357959793	8.51249590904825
H	31.73604441278470	-26.45451532861480	6.75028094186854
H	31.08357056984597	-28.05810509162366	6.31045907600359
H	31.80179827827788	-27.81424003022135	7.89673854479501
H	32.63102486387940	-26.20794667290906	1.59737378446998
H	36.91830975079610	-26.65790560148998	9.46955560956610
H	37.47306381046860	-29.64780357387406	3.87768705488866
H	32.25316850298915	-23.02424557250751	7.10482098529180
O	36.02120549360999	-25.20625491661173	4.93228189628641
H	35.63442374184536	-24.32708604891965	5.06014489987586

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B3LYP Scan/Hydroxide IPC Model/RKS/2.4 Angstrom Fe-C Bond Length Constrained Optimization

C	30.89645589024150	-24.19098725952473	2.10056564477682
C	35.63224650458443	-24.70531542157224	10.83467813846087
C	39.09661697979606	-30.05179254369311	6.03373741772294
C	33.98365365575855	-28.10875891704960	0.20101659800719
N	33.29173766448368	-25.28208225354891	4.78419602602718
N	34.64074983767716	-25.42666329595428	7.28282251079620
N	34.94323294518282	-27.40787840465351	3.76510982440526
C	33.16620827581686	-26.25470997633366	2.53987543922420
C	32.85664135969706	-23.84984346643781	6.72343050024322
C	36.41035985357586	-26.59333389661443	8.51111695716868
C	36.82663383561616	-28.87735826148354	4.27819072575346
C	30.69658432918489	-22.56527643359735	4.91052067401581
C	33.25197308009717	-22.84142329782854	9.63208981335530
C	38.77591671186200	-28.55342190921153	8.90733607768593
C	36.46379417977879	-29.86366263307904	1.36053517142531
C	32.75647942020085	-25.36402811844937	3.52819132396595
C	33.79552634024263	-24.39766859873826	7.59410778690192
C	36.84163707360215	-27.46022081412880	7.51147244071291
C	35.84557701682781	-28.37553793906030	3.43009891841300
C	31.69855561771060	-24.37820046940861	3.35475103602344
C	34.01022477873657	-23.95031800129795	8.96344488809871
C	37.95717955410094	-28.38806067666988	7.66071577774627
C	35.65025625026682	-28.80948060230922	2.05145675734765
C	31.61450172953778	-23.69169451209102	4.53646700900465
C	35.01152586518484	-24.73444542999942	9.46923906392360
C	38.08850740872872	-29.02335431142406	6.45557942107348
C	34.60887884669818	-28.07144808293548	1.56352389786760
C	32.61962786522994	-24.26948598230567	5.41637326297781
C	35.39720176419979	-25.64645146944880	8.40044436761109
C	37.04224738040044	-28.48255328707907	5.59577688947207
C	34.18753212102041	-27.19273258095648	2.64955496148969
N	36.30612076026037	-27.54640858661214	6.25944624747749
Fe	34.79600101623289	-26.42227009151348	5.51890348256761
C	34.19564127926184	-31.34194014758512	7.44605957103303
C	35.42980855857341	-31.78977422533485	6.67936087880376
C	31.87929652420614	-27.50868564323541	6.88986747715458
C	33.17035457744258	-27.98682058742455	6.33710602254905
C	33.30643777450608	-29.43088072940991	6.32726145599764
O	32.84250514743482	-30.15029468821488	5.45878937085430
O	34.02151692769123	-29.91376760004425	7.38854347995943
H	29.98913983338513	-22.33614142473921	4.10550692628371
H	31.24916548071051	-21.64072273121449	5.13169338765208
H	30.10564752076920	-22.80133914298784	5.80670151417474
H	31.52221722549533	-23.86076951077228	1.25880914354221
H	30.40882571176476	-25.12384023300086	1.78514232518147
H	30.10968370121931	-23.44012534826324	2.23463331431796
H	34.02897671693310	-27.12942879657168	-0.29634779850904
H	34.48651998137748	-28.82992617897999	-0.45285554494012
H	32.92264913372608	-28.39267689034205	0.24669066687273
H	36.17177206803133	-29.97326861183867	0.31004729218268
H	37.53670857430249	-29.62644326824577	1.37812110589060
H	36.34837180878743	-30.84801334260253	1.83607816822018
H	33.57974749743720	-22.69653217088452	10.66765929045987

H	32.17127133675297	-23.04145032764190	9.65633571056733
H	33.38340134713126	-21.88268622037382	9.11037129735103
H	36.70859800718240	-24.48677414406338	10.78904670746564
H	35.52823024794054	-25.66990467403732	11.35154442978494
H	39.57265443186097	-29.29309259906775	8.76978771332490
H	39.25291216144404	-27.61094299930628	9.21156952169295
H	38.16421348099245	-28.88750800698896	9.75758999904871
H	38.62175872973782	-30.99813237588988	5.73826517446408
H	39.68577701963152	-29.71059161995718	5.17093275818617
H	39.80249286086085	-30.28060497262165	6.84048737267464
H	35.17055838200020	-23.94258573562603	11.47171287061506
H	36.31752087812295	-31.26902385283091	7.04435853874483
H	35.57788995184293	-32.87006323960107	6.79721691091047
H	35.31781947736526	-31.56727822893208	5.61704822626043
H	33.29794028169796	-31.82798618330144	7.05735238595584
H	34.28946533323518	-31.56332601413310	8.51243110079522
H	31.70386554961195	-26.45056241710178	6.70347453745222
H	31.03318442247851	-28.10034246498659	6.50264740238471
H	31.87651276352268	-27.66520690834774	7.98417592190316
H	32.64975919142064	-26.19970878582321	1.58569230431765
H	36.92955579754257	-26.64631649756982	9.46408424820078
H	37.48648209995193	-29.64056140015206	3.87517660604129
H	32.25080523729333	-23.03016606388869	7.09944024325028
O	36.04746234367364	-25.18364475793543	4.92822020905130
H	35.66021597511162	-24.30571310511698	5.06386762213160

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B3LYP Scan/Hydroxide IPC Model/RKS/2.5 Angstrom Fe-C Bond Length Constrained Optimization

C	31.05402797892968	-23.95001936347867	2.01808283154154
C	35.53161521472229	-25.10942900271522	10.82462598518974
C	39.10033953047125	-30.13813488604876	5.74301953809219
C	34.08736904404923	-27.85159379294719	-0.02937325146529
N	33.33682745004868	-25.29901136927866	4.68423542852768
N	34.57252664008821	-25.67169467063585	7.23562765855519
N	34.99498205730254	-27.33984639237952	3.58408875906057
C	33.29297309175787	-26.06988048815469	2.36375613924888
C	32.76115121066583	-24.10485544038827	6.74759056811465
C	36.42685807537724	-26.78453828550676	8.37540123491539
C	36.80725361154201	-28.91321054699772	4.06076804309330
C	30.69946157859524	-22.63333400508809	4.97159630474354
C	33.03912811522934	-23.32211186857993	9.73647633820928
C	38.87135587630636	-28.66795789044385	8.64314088379275
C	36.43713231294922	-29.78739932311953	1.11790635401726
C	32.85507538060499	-25.25384455936637	3.40387756000528
C	33.68138121008501	-24.70501356688242	7.60393360040799
C	36.87453664123618	-27.58546995827691	7.32942418205422
C	35.85768685439452	-28.34206464273347	3.22582128390963
C	31.79897730692546	-24.26196645505437	3.28293728615033
C	33.86256211851420	-24.34028465261661	9.00403008202841
C	38.00708767035697	-28.49751531268399	7.42799873084063
C	35.66783988927637	-28.71390118283816	1.82959234035848
C	31.64768282525212	-23.70829454116948	4.52780367134614
C	34.91215958347080	-25.08990844197149	9.45901064496075
C	38.10471061684083	-29.11758210242509	6.21081920130319
C	34.68146151075494	-27.90062850090946	1.34693619671767
C	32.61410285824197	-24.36892163306725	5.38855315606710
C	35.35093880675682	-25.90687566408748	8.33429524895298
C	37.03612185995178	-28.56461259729108	5.38968076226617
C	34.27710554789488	-27.04556000781839	2.45579257464948
N	36.30942206783209	-27.64814109939620	6.08805304094899
Fe	34.81730411814105	-26.49108674827812	5.38490234037895
C	34.48311022502802	-30.57195958749469	8.52649935774110
C	35.37040130595984	-31.48589476971537	7.69364601566237
C	31.69104081200256	-27.49390053305309	6.35021900928958
C	33.06159695389393	-28.04843489916436	6.24638889034993
C	33.25474229486938	-29.30046792838072	6.93836139205923
O	32.60884936418572	-30.30485263297005	6.64712967673575
O	34.24032682681849	-29.31457047824554	7.87645799056849

H	30.01922795224111	-22.33764749728856	4.16500839426228
H	31.22980106861501	-21.72725434696258	5.29861270484731
H	30.07947714823489	-22.95922635279793	5.81833037294472
H	31.71293188131929	-23.52676654976069	1.24611820835219
H	30.59528467586644	-24.84913516806196	1.58377547470100
H	30.25030963537202	-23.22604103639943	2.19231904567401
H	34.22640101038636	-26.86813115760085	-0.50080472494755
H	34.54153262774264	-28.59737193453580	-0.69109472129749
H	33.00527476726642	-28.04371975052453	-0.01265603430306
H	36.12599602219794	-29.87928975908620	0.07129520018427
H	37.51759350777355	-29.58560076484480	1.12116858031705
H	36.29687972872127	-30.77015954070764	1.58934134426528
H	33.32964911817371	-23.25178924598923	10.79066319926508
H	31.96780239767678	-23.56611619369842	9.70856782236506
H	33.14546311078502	-22.31808980997037	9.30097294996459
H	36.59243049498886	-24.82288887142735	10.79534748355960
H	35.48576758703494	-26.10908594709642	11.27929862984772
H	39.67438645105486	-29.39224030130936	8.46620101720157
H	39.34399958668781	-27.72196896276705	8.94271352007880
H	38.29750927912935	-29.02384820186107	9.51066751455759
H	38.61314102937754	-31.07434153917526	5.43550230652770
H	39.67308702251003	-29.77889057245599	4.87639666089613
H	39.82108982581168	-30.38966715768435	6.52931972308100
H	35.02533681652349	-24.41719324591273	11.50658914139860
H	36.30962350287942	-30.98591962201520	7.44840160090419
H	35.59439211967697	-32.40500255002839	8.24890790941265
H	34.86490294580223	-31.75646662273726	6.76568277021093
H	33.52764143680674	-31.05539325150807	8.74748448030156
H	34.97164354167489	-30.29886106040189	9.46488528431483
H	31.38766889641598	-26.96607714562988	5.44263252777964
H	30.94121645431049	-28.24975422706745	6.62232043815040
H	31.69144007965861	-26.72558104536620	7.14358516186911
H	32.81327475609640	-25.94006751681762	1.39779381073516
H	36.97004359104624	-26.85296591714948	9.31398461100084
H	37.44251948744418	-29.68341142260156	3.63270335142222
H	32.11812521940561	-23.34007452225943	7.17424281701242
O	36.08451304270277	-25.17250439740586	5.07626530362245
H	35.59911500725902	-24.34911936143526	4.91481598012959

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Hydrogens Only Optimized PDB 6CUN Crystal Structure

C	38.34163172145838	-22.38738249371318	4.96658446554173
C	37.36461887443744	-23.53183320829774	4.84610379637233
C	37.00845233841009	-24.51845612058054	5.71742280304463
N	36.59168459058323	-23.72541236596193	3.70279022409523
C	35.78733725891380	-24.75706751092958	3.93855233228817
N	36.00819068866760	-25.24549310703418	5.15370886203537
C	30.26539695255331	-25.28433397725444	3.01048519108334
C	36.07284249659648	-24.23468844196876	11.01678275441978
C	39.78607040585492	-29.52036667264952	6.35660421069090
C	33.76428931086832	-29.01131481868801	1.03642849848707
N	33.17537756824233	-25.84382128350323	5.38779344738214
N	34.76688451520101	-25.59746636004419	7.69926652572795
N	34.96717237168055	-27.74747986062414	4.40010458577548
C	32.85768122916617	-27.07547129583082	3.30118041420742
C	32.83251636629829	-24.23242795237114	7.16581128687918
C	36.65616113939028	-26.54674791361891	8.92780530604104
C	37.11431825466166	-28.84220043899744	4.73908856531143
C	30.24494222332521	-23.50219559047607	5.70399343727821
C	33.55134337723883	-22.67218187238918	9.71396419488286
C	39.28928809934580	-28.08918719988645	9.20647379270315
C	36.64827137653437	-30.15407483675417	2.00954530616126
C	32.46906258046522	-26.11586643490497	4.23024311577862
C	33.90533472770281	-24.53252966417230	7.94364627615662
C	37.12492599911027	-27.36849849897164	7.94113811309496
C	36.01254419489084	-28.60037745195211	4.00232539934237
C	31.28066554987706	-25.28058274481093	4.15813433518472
C	34.27145243017670	-23.89112947533603	9.17277474897841

C	38.37063557270104	-28.10709709284032	8.00541828877125
C	35.69441257859141	-29.16664621095133	2.72674915483755
C	31.28842824851669	-24.53265897931124	5.26990951169717
C	35.31438627715595	-24.54099676266593	9.69806153651062
C	38.50689864485010	-28.73156527935781	6.82484854190555
C	34.52366368701481	-28.68042359283506	2.32776939121401
C	32.47299450081388	-24.83971811362173	6.01113495413807
C	35.64966845306442	-25.61123829464716	8.78101364678175
C	37.35193943371704	-28.42357055679255	6.02041307711521
C	34.03951366351754	-27.78280676731824	3.36739272686727
N	36.52158548642179	-27.55672230096931	6.72965714003229
Fe	34.85354922074428	-26.69070877987376	6.06404866458603
C	32.13240438006077	-30.55970583000973	4.98777283143274
C	31.07908538502526	-31.33599198038723	5.71431601351679
C	33.18331301366169	-27.79695650603030	8.42972787181651
C	33.82018504255905	-27.96182887718512	7.07399671994363
C	33.58978979462267	-29.23998350712057	6.49173461942085
O	34.35904253315750	-30.17520762355089	6.60102468735890
O	32.39553894859998	-29.35822080588829	5.73200820796991
H	32.22571129480894	-27.22051086609135	2.42101423722855
H	37.86132704732609	-29.51652588464284	4.30710627192039
H	37.24260546283313	-26.49237373128095	9.85060769561257
H	32.18814494285662	-23.41798177982878	7.51249207202606
H	37.36751050144850	-24.71417573164113	6.72322640486695
H	35.04776784823849	-25.14172167057372	3.24250643512964
H	36.61484815167994	-23.15162935065670	2.86550344776249
H	37.83652990099992	-21.40811206658685	4.90774777421006
H	39.11985475059520	-22.41186757209915	4.18449750808474
H	38.85104144337899	-22.43597458148557	5.93879711811749
H	29.78093064490514	-26.26877190426462	2.89824600492131
H	30.74744172331210	-25.04602316019124	2.04756327892860
H	29.47301305992920	-24.54156191961448	3.17677784646609
H	30.67872550903498	-22.49230375670024	5.80107925359934
H	29.42118669202282	-23.43760484670675	4.97965712835637
H	29.80460082510584	-23.76221582536246	6.68102138495095
H	33.99688496991636	-22.32037347181469	10.65534283687924
H	33.58339710734542	-21.83121589353391	9.00060933354916
H	32.48682336202526	-22.88154035267549	9.91660460114880
H	36.04486418341777	-25.09680045972794	11.70313801787197
H	37.13243160273521	-23.99982904539795	10.82374425258761
H	35.62699768829296	-23.37688402216227	11.53835471496252
H	40.14273321329402	-28.76968401380622	9.07654412140607
H	39.69931930150664	-27.08210001502553	9.39617588514046
H	38.76246465199709	-28.40166964969647	10.12374443550823
H	40.29782725766051	-28.98140180287073	5.54297102684055
H	39.53080963458448	-30.52614613556508	5.98634713605771
H	40.49225880416357	-29.63547801594808	7.18894592903340
H	37.63398868981542	-29.69473325364024	1.82966289097427
H	36.24487912590597	-30.46979885990176	1.03726516082896
H	36.80832603298091	-31.05975390045166	2.61642521627540
H	34.32563329765327	-29.72530470248043	0.41811471405436
H	33.58641995768114	-28.11054771096577	0.42478108266072
H	32.77881914230478	-29.45864884718621	1.24915989239361
H	32.50182051347137	-28.62295420986440	8.68957341768295
H	32.64001806318703	-26.84016765092350	8.48124332999002
H	33.96889123902361	-27.73381079182946	9.20459216658971
H	31.79770909646294	-30.22076449312720	3.99501363372422
H	30.18637952333362	-30.71579744703310	5.89067886649657
H	30.76604450596641	-32.22417771890965	5.13844624483839
H	31.45157415349078	-31.68450803183761	6.68999859642880
H	33.06640817085750	-31.13287074481752	4.87441994103363