

DFT OPTIMIZED STRUCTURES FOR CHAPTER 2: QUANTIFYING ENTATIC
STATES IN PHOTOPHYSICAL PROCESSES: APPLICATIONS TO COPPER
PHOTOSENSITIZERS

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Bis-phen reduced

Cu	-0.00000045180095	-0.00000082557986	0.00000200948944
N	-1.47545351489826	0.94105946029493	-0.94091794975745
N	-1.47545302335271	-0.94106019759545	0.94092202116185
N	1.47545218199328	-0.94106263171841	-0.94091630714409
N	1.47545259488265	0.94106441756805	0.94091627470558
C	-1.45208263948285	1.89203832852108	-1.89173212355800
C	-2.61871982472391	2.45193690228207	-2.45151957393734
H	-2.52790059905708	3.22243151246017	-3.22188624793560
C	-3.86784423663454	2.01556659384930	-2.01521561942959
H	-4.78861776541730	2.43444277923660	-2.43401520823286
C	-3.93864027168419	1.01370382866639	-1.01352428673883
C	-5.17021433402305	0.48623940286775	-0.48614962541675
H	-6.11568543721488	0.87672629129434	-0.87656608663094
C	-5.17021407638896	-0.48623992681920	0.48615555127564
H	-6.11568498360864	-0.87672680579170	0.87657247766824
C	-3.93863976934918	-1.01370439792311	1.01352959898990
C	-3.86784329755497	-2.01556714914112	2.01522094286770
H	-4.78861659689172	-2.43444332545003	2.43402106664306
C	-2.61871868130798	-2.45193752710443	2.45152425385507
H	-2.52789910513559	-3.22243212286204	3.22189089318130
C	-1.45208175643119	-1.89203908338911	1.89173621980103
C	-2.70574329987752	-0.50843025537852	0.50834857009951
C	-2.70574354644548	0.50842961576999	-0.50834391228628
C	1.45208091820129	-1.89204514207900	-1.89172685264853
C	2.61871783009797	-2.45194454160570	-2.45151398346919
H	2.52789828966388	-3.22244217303315	-3.22187761103305
C	3.86784242128642	-2.01557125325026	-2.01521352255066
H	4.78861575433081	-2.43444808868220	-2.43401288128277
C	3.93863890543006	-1.01370459859614	-1.01352610304279
C	5.17021319185022	-0.48623696491471	-0.48615520766887
H	6.11568409456427	-0.87672444222625	-0.87657153306059
C	5.17021340688604	0.48624603044971	0.48614629452398
H	6.11568450813993	0.87673526697426	0.87656040134490
C	3.93863935649257	1.01371133673460	1.01352007354012
C	3.86784333158909	2.01557789486182	2.01520762414895
H	4.78861680835056	2.43445655479721	2.43400484594573
C	2.61871889791583	2.45194874471527	2.45151099727074
H	2.52789966186213	3.22244623062862	3.22187479069022
C	1.45208172236709	1.89204694603063	1.89172681288250
C	2.70574266259741	0.50843411421784	0.50834267382596
C	2.70574242556743	-0.50842972787920	-0.50834582679873
H	-0.46002389589419	2.21959452123800	-2.21924809085886
H	-0.46002288691821	-2.21959536644684	2.21925169987222
H	0.46002299814592	2.21960346898375	2.21924250086029
H	0.46002203187850	-2.21960369497599	-2.21924004116217

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Bis-phen oxidized

Cu	0.0000008958897	-0.00000026105731	0.00000079777961
N	-1.49020989721903	-1.25770298576355	0.43893145622942
N	-1.49020892390928	1.25770299655776	-0.43893250410459
N	1.49020933977710	1.25770408665772	0.43892927621142
N	1.49020975572575	-1.25770478842542	-0.43892646329825
C	-1.44192103994374	-2.48766958450554	0.97383549946023
C	-2.60903615288589	-3.20813431403379	1.31111935462361
H	-2.51281701103057	-4.20675806507391	1.74482873093613
C	-3.85863785121835	-2.63933509723779	1.08029559627631
H	-4.77420135419087	-3.18966767509960	1.32020896542112
C	-3.94210405583558	-1.32930390474165	0.53595643330840
C	-5.17477878415583	-0.63600339188888	0.26287733537152
H	-6.11992711599581	-1.14428342420101	0.47714162132167
C	-5.17477819711051	0.63600376220295	-0.26288579313877
H	-6.11992607537637	1.14428382603681	-0.47715200668200
C	-3.94210286851416	1.32930417230384	-0.53596235528891
C	-3.85863546229868	2.63933540133723	-1.08030126914668
H	-4.77419843425254	3.18966809538674	-1.32021639207972
C	-2.60903325402684	3.20813448516596	-1.31112252761902
H	-2.51281312651530	4.20675824769851	-1.74483166510899

C	-1.44191889081664	2.48766959813777	-0.97383640104021
C	-2.71308217469842	0.67008637367672	-0.25269716324917
C	-2.71308272928738	-0.67008622772467	0.25269369279038
C	1.44191963973952	2.48767239116430	0.97382931086698
C	2.60903423928532	3.20813836753258	1.31111229467469
H	2.51281442313041	4.20676350344574	1.74481834470963
C	3.85863629961224	2.63933857026130	1.08029191910301
H	4.77419942425491	3.18967205985865	1.32020463900747
C	3.94210336623645	1.32930562022731	0.53595709010180
C	5.17477851995957	0.63600436415237	0.26288177658185
H	6.11992654162033	1.14428515761761	0.47714562378638
C	5.17477875197810	-0.63600448248574	-0.26287727006073
H	6.11992696009277	-1.14428512660759	-0.47714065257424
C	3.94210383518897	-1.32930591632686	-0.53595313205282
C	3.85863725680992	-2.63933891162455	-1.08028790346086
H	4.77420063288858	-3.18967218273915	-1.32020015470512
C	2.60903541327640	-3.20813895525836	-1.31110880438720
H	2.51281594318811	-4.20676414061534	-1.74481481223894
C	1.44192054000276	-2.48767314525358	-0.97382639889652
C	2.71308270509239	-0.67008735544264	-0.25269160402639
C	2.71308248235189	0.67008688401383	0.25269491224587
H	-0.44869701847184	-2.91381692416865	1.14242616412654
H	-0.44869451226049	2.91381685474839	-1.14242506357200
H	0.44869641359050	-2.91382111116883	-1.14241484932962
H	0.44869535662317	2.91382015326030	1.14241735112670

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Bis-phen triplet

Cu	0.00000582844822	-0.00000011576791	-0.0000007570708
N	-1.47262723120285	1.26092696364568	-0.40408627900386
N	-1.47262652994161	-1.26092713059245	0.40408813608149
N	1.47262687504893	-1.26092446428898	-0.40409038431679
N	1.47262675658106	1.26092513049082	0.40408860688520
C	-1.43223904291569	2.50139309300523	-0.93647883294918
C	-2.58941650509857	3.22253237913189	-1.26536524302676
H	-2.49017963871177	4.22593862269329	-1.68670345350509
C	-3.85324993852060	2.65227408144878	-1.04113258948092
H	-4.76704983716610	3.20810961455779	-1.27305369237175
C	-3.93549905172112	1.34262011154681	-0.51956477055236
C	-5.16567753475693	0.63890255555460	-0.25435356746043
H	-6.11185463772115	1.14934462648462	-0.46141297604447
C	-5.16567708343223	-0.63890293144586	0.25436131274144
H	-6.11185381401402	-1.14934511541982	0.46142216065281
C	-3.93549813916945	-1.34262039163800	0.51957056865959
C	-3.85324816292378	-2.65227439606220	1.04113817127658
H	-4.76704766838721	-3.20810998889867	1.27306069684496
C	-2.58941435246598	-3.22253265990948	1.26536874863560
H	-2.49017673653000	-4.22593892356747	1.68670673599385
C	-1.43223746883243	-2.50139329629943	0.93648052243680
C	-2.70923350708346	-0.66776780914459	0.23808553699905
C	-2.70923392671751	0.66776763172120	-0.23808163233325
C	1.43223778545269	-2.50139001108445	-0.93648546076688
C	2.58941453127029	-3.22252881575400	-1.26537419229893
H	2.49017650572190	-4.22593420494322	-1.68671417437772
C	3.85324897713396	-2.65227167816167	-1.04114217807032
H	4.76704815684276	-3.20810741475376	-1.27306554082984
C	3.93549935442047	-1.34261873321195	-0.51957231777213
C	5.16567798721330	-0.63890110723197	-0.25436148658040
H	6.11185488650180	-1.14934271547522	-0.46142295493090
C	5.16567799323836	0.63890363788971	0.25435538840757
H	6.11185489441662	1.14934570699560	0.46141575502401
C	3.93549932993371	1.34262063721076	0.51956764538051
C	3.85324892094049	2.65227349818158	1.04113770495186
H	4.76704808752149	3.20810968282720	1.27306004723145
C	2.58941445164844	3.22252995233273	1.26537128759831
H	2.49017637271448	4.22593523023990	1.68671150180854
C	1.43223769115941	2.50139057349742	0.93648388523926
C	2.70923490729970	0.66776779888727	0.23808296493564
C	2.70923493848512	-0.66776647832580	-0.23808627812349
H	-0.43731921144101	2.92575026142647	-1.10038621260117

H -0.43731737056599 -2.92575046285288 1.10038623316400
H 0.43731753130960 2.92574629034232 1.10039273881758
H 0.43731762601665 -2.92574623528187 -1.10039305666233

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Bis-phen* reduced

Cu 0.03749898827072 -0.02983134399214 0.18529707990542
N -1.44537021158701 1.01914471808885 -0.61953075565935
N -1.43097452564820 -1.13836409208707 0.93797797107757
N 1.46925087017854 -0.97020757845355 -0.85174261744901
N 1.55503851463339 0.84611414173091 1.09238253502418
C -1.42911785807214 2.11518299420079 -1.39803802390084
C -2.59975081359889 2.74988477056092 -1.86124908245662
H -2.51444500790537 3.63643647175891 -2.49557628673909
C -3.84566327844477 2.23368124177279 -1.51097939427761
H -4.76976465999999 2.70449618706965 -1.86201035871168
C -3.90838506431362 1.07872019739399 -0.69015985839454
C -5.13565772775803 0.45225866435715 -0.27222097791896
H -6.08406359920796 0.89045198138331 -0.60019215134955
C -5.12801443238378 -0.67417083766911 0.51638255023196
H -6.07018232388881 -1.14114917744942 0.82179069292607
C -3.89239398771602 -1.26644371417063 0.95887255495202
C -3.81377468495016 -2.42616631747717 1.77159132071133
H -4.73115602487428 -2.92639129372258 2.09873021185838
C -2.56120108138754 -2.91204481862566 2.14107197819129
H -2.46395509523877 -3.80311014174833 2.76727078519970
C -1.39970454549276 -2.24108584129545 1.70697320454721
C -2.66390779034489 -0.66088908347400 0.56548709183419
C -2.67171014885209 0.51135789807719 -0.26688379578210
C 1.39966059928567 -1.89655448890576 -1.82291697929707
C 2.53874026316122 -2.45666736254205 -2.43738647552321
H 2.41147214735630 -3.20501902253237 -3.22435190729251
C 3.80744651706488 -2.04307156800960 -2.03688230579134
H 4.70781927343842 -2.45924490638835 -2.50059511966027
C 3.92634109496743 -1.06759896361295 -1.01391852667198
C 5.18150670317378 -0.56160051373210 -0.52283219069113
H 6.10826786517121 -0.94912946551924 -0.95857977344777
C 5.22538946163890 0.38915756921735 0.46976420519040
H 6.18799114466895 0.76567868503201 0.83132365380852
C 4.01933039573331 0.91062886822558 1.05880287328097
C 3.99440964613732 1.88693502476638 2.08756754157418
H 4.93418283594536 2.29132291471555 2.47795952988788
C 2.76571688022404 2.31354720900304 2.58557139958320
H 2.71177201588769 3.06275793689281 3.38043994042106
C 1.56786806240132 1.77370475842007 2.06955239349461
C 2.76410853346852 0.42377511193007 0.59355812144642
C 2.71782644780755 -0.56437599177597 -0.45016795091358
H -0.43930349476482 2.49968268585091 -1.66507483348546
H -0.40504506013765 -2.60110796330176 1.98967784755344
H 0.58801775122138 2.09014352478374 2.45461376987896
H 0.39204692672637 -2.20174177396131 -2.12410334971585
O -1.34782341295118 2.61519195070730 3.25444450921459
H -1.59067055995578 3.56209221843593 3.23191758273001
H -1.46572342408781 2.36860667907138 4.19327599860590

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Bis-phen* oxidized

Cu 0.04705814370317 -0.00659704630282 0.51623515635170
N -1.48291969580691 -1.27552855577481 0.68614863017106
N -1.42406536789932 1.25811511829478 -0.17139329662965
N 1.59714604171878 1.22971722451505 0.69730371177418
N 1.46548028125305 -1.26637384466833 -0.21052995774874
C -1.48541827816376 -2.50953480062964 1.21301242240976
C -2.65908867785678 -3.28989422735731 1.29846825388702
H -2.60654402245590 -4.28974403485809 1.73695137158990
C -3.85968938258115 -2.77563189454622 0.81592797607058
H -4.77773536482556 -3.37074214317723 0.85816138894220
C -3.89271903824335 -1.46318346534318 0.27319791223146
C -5.07805751885118 -0.82729310441760 -0.24045783674466
H -6.01922878147356 -1.38555000624759 -0.22855357500075

C	-5.03654271605769	0.45395544231633	-0.74017184848882
H	-5.94426595159563	0.92140637307884	-1.13427885094109
C	-3.81171465655341	1.21176329248573	-0.74992179142984
C	-3.69862089911531	2.54043726152192	-1.24076087837805
H	-4.57885380470973	3.04833525673967	-1.64802946719043
C	-2.46417597386655	3.18037195915106	-1.19967506765533
H	-2.34170052840162	4.19844207516941	-1.57811814024658
C	-1.34837719302391	2.50489419292728	-0.65521388039627
C	-2.62708287244785	0.60858708367454	-0.23904347287795
C	-2.66435121674007	-0.74123268879350	0.24775631061868
C	1.62200304188635	2.45665201565294	1.23896793078200
C	2.80940922107456	3.21867877555473	1.31032365503614
H	2.77848039433803	4.21518741747999	1.75843521702632
C	3.99701691885384	2.69130687702832	0.80911388231802
H	4.92426638776671	3.27226937364460	0.84677985319734
C	4.00387116992604	1.38329156244726	0.25433554199073
C	5.16925302223624	0.72692957958259	-0.27938932347860
H	6.12338846971347	1.26275947625918	-0.27046170550971
C	5.09321958822379	-0.54643177933844	-0.79583667160464
H	5.98593223016264	-1.02901305438291	-1.20551912346805
C	3.85060690966544	-1.27521813424692	-0.80742540643523
C	3.69618262201999	-2.58888427560579	-1.32552012333326
H	4.55804361485942	-3.11358072007536	-1.75033842594516
C	2.44258293681705	-3.19193412564744	-1.29286627285014
H	2.28688767883536	-4.19610183730582	-1.69541036964420
C	1.34958426635131	-2.49919630852823	-0.72624303203866
C	2.68849187776050	-0.65176923267425	-0.27169732949282
C	2.76311319952863	0.68577241228579	0.23594554598331
H	-0.52716891237355	-2.88802811843998	1.58235292364135
H	-0.36943065436069	2.99121465891806	-0.60963202473350
H	0.35640248825049	-2.95537929419560	-0.69299625429153
H	0.67514281278516	2.82452006519885	1.64367424950589
O	-0.45968089912125	0.70178377926865	2.74443716576887
H	0.10669842983053	0.55810933158160	3.53081124417133
H	-1.37005412903584	0.73295745677986	3.10316833708588

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Bis-phen* triplet

Cu	0.01419458183745	-0.02044351059375	0.39404010975106
N	-1.44859352417369	1.25426922784065	-0.17807341039078
N	-1.48986956575647	-1.28795411958585	0.59195313726005
N	1.45680181698471	-1.28951530359124	-0.19374438124692
N	1.52909650092542	1.22621479369995	0.61942728293294
C	-1.37991839054307	2.50805520372914	-0.66207871650963
C	-2.49988254583949	3.20474414039122	-1.14635432052837
H	-2.37603047881747	4.22544851040205	-1.51652986032573
C	-3.75762197507345	2.58409751764226	-1.13886279350673
H	-4.64636186591541	3.11391927398054	-1.49622531816323
C	-3.86799931254373	1.25779449681635	-0.66862521903596
C	-5.09759023339649	0.50864506998369	-0.61553594614783
H	-6.01770859683438	0.99266452117514	-0.95913150279394
C	-5.13074154439207	-0.78123450046675	-0.13964204818918
H	-6.07820455484452	-1.32836942568130	-0.09678750643178
C	-3.93343421287884	-1.45030036068150	0.30579289877781
C	-3.89216050409342	-2.76892877490544	0.81056826937978
H	-4.81202027694380	-3.35749850660438	0.88162330509789
C	-2.66053081738023	-3.30494578083411	1.22667123155525
H	-2.59629094377198	-4.31439925591572	1.64073276859293
C	-1.49301913567097	-2.54038173967230	1.10155251666711
C	-2.70212503226508	-0.72962218648970	0.23431274436218
C	-2.67341043670820	0.61714636264078	-0.21396829108064
C	1.37244274488309	-2.53261134345726	-0.71051289781777
C	2.48240071633541	-3.22739616367888	-1.21589666362342
H	2.34458590362133	-4.23699923500748	-1.61086948203839
C	3.74865384192845	-2.62214613705193	-1.19999736417561
H	4.62918273196326	-3.15387132069105	-1.57405625098116
C	3.87435679024243	-1.30695580374814	-0.70296015840366
C	5.11018580888653	-0.56669121708707	-0.64554600411525
H	6.02377163127888	-1.05198084092312	-1.00432219810111
C	5.15754242628845	0.71536021563173	-0.14976322293374

H	6.10974230371170	1.25408244750905	-0.10604859851920
C	3.96848609218845	1.38519491702038	0.31516411283959
C	3.93239972293548	2.69618826548591	0.83967572962584
H	4.85371859373419	3.28260060406234	0.91190417092542
C	2.70690092200241	3.22684832240046	1.27650349182939
H	2.64986204366072	4.22873791906895	1.70956376801362
C	1.53465434243750	2.46559044643830	1.15361155793422
C	2.73387569203359	0.67179412349972	0.24327321726209
C	2.69015728500208	-0.66604992693831	-0.22602219333583
H	-0.39042415311755	2.97515138309707	-0.65644728705913
H	-0.52234471365257	-2.93375994497448	1.41909160489669
H	0.56814204956308	2.83693348283593	1.50512469721331
H	0.37758616943406	-2.98706813317569	-0.71736186013403
O	-0.47215517275479	0.63447319132393	2.76543726178702
H	0.12621063766929	0.46751741869566	3.52137229676500
H	-1.36597325218032	0.44885559838425	3.11650198911981

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Bis-mmp reduced

Cu	-0.00000082563352	-0.00046025044141	-0.27061331626738
N	-1.54657317651021	-0.97061779929675	-1.04350957694932
N	-1.42798883004183	0.97723011098391	0.77278889663983
N	1.427976832282563	-0.97433425380988	0.77637320959390
N	1.54657894053497	0.96684060419398	-1.04705352601664
C	-1.55572356122574	-1.96459285209576	-1.95768243519515
C	-2.76944601931816	-2.57605339134087	-2.36525823344863
H	-2.73514452463599	-3.37636464174703	-3.11045358181519
C	-3.98293587252315	-2.16177929775630	-1.82982687710399
H	-4.92221768599083	-2.62894808303509	-2.14368827692606
C	-3.99865327153014	-1.12042308767232	-0.86516216855787
C	-5.19139445137194	-0.61112513902217	-0.24226816356870
H	-6.15573207635276	-1.04596757863868	-0.52494974855831
C	-5.13198350561958	0.39914729491251	0.68953632867572
H	-6.04799682309098	0.77638193053299	1.15579239378776
C	-3.87365850245534	0.98055548869874	1.07582703726467
C	-3.73967683738977	2.01709581756962	2.03552390072348
H	-4.63019766382196	2.42314544948001	2.52646489692696
C	-2.47033738037536	2.50230085566659	2.33956764248433
H	-2.33175958768189	3.29884956745201	3.07568791908388
C	-1.34410204754523	1.95619956442712	1.68850596593421
C	-2.67692148701882	0.49409584500356	0.47144418365448
C	-2.74187134708035	-0.55976259310404	-0.50516566864709
C	1.34408110365789	-1.94994862057535	1.69566306209733
C	2.47031472967668	-2.49369878093754	2.34869274057830
H	2.33173055036956	-3.28755292657378	3.08771692147446
C	3.73966063537244	-2.00963734509348	2.04285851829272
H	4.63018003571120	-2.41391439480302	2.53526279589327
C	3.87365094670705	-0.97660786917975	1.07938455813267
C	5.13198190915283	-0.39663392251918	0.69096259588316
H	6.04799395793957	-0.77218119909292	1.15858131795237
C	5.19139907201080	0.61023641274732	-0.24451671840582
H	6.15574042305013	1.04403296913668	-0.52878794392414
C	3.99866069393478	1.11727596361563	-0.86925566374173
C	3.98295073693739	2.15510998190412	-1.83770852302907
H	4.92223580705356	2.62112482509589	-2.15327104857024
C	2.76946353224969	2.56743824837969	-2.37464592136124
H	2.73516719463826	3.36502959379865	-3.12275190432483
C	1.55573696268358	1.95747447061201	-1.96484592989513
C	2.74187407509425	0.55794588442855	-0.50721158869064
C	2.67691585231760	-0.49233463937561	0.47324432413507
C	-0.22417728199720	-2.38329917319419	-2.52114820294824
H	-0.19122558213656	-2.25285953814396	-3.61747226831427
H	0.56708448612955	-1.76858234270132	-2.06235042270824
H	-0.01493982545495	-3.44765736742872	-2.31278602870255
C	0.22419343185566	2.37413175912701	-2.52983553782295
H	0.19126066272963	2.23975740120618	-3.62568432905320
H	-0.56706637863257	1.76105749200489	-2.06884141831963
H	0.01493587280735	3.43922826616640	-2.32529878225845
H	-0.33603903063847	2.32192628961543	1.91040091300573
H	0.33601226017326	-2.31483249118035	1.91891491291042

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Bis-mmp oxidized

Cu	-0.0000194636059	-0.00090349164189	-0.45686283367127
N	-1.53415755945926	-1.21601281798609	-0.84208221356380
N	-1.42845162199043	1.21306401857292	0.26412096423668
N	1.42845127454759	-1.21241030630722	0.26824061579091
N	1.53414542140134	1.21291447801891	-0.84615808072237
C	-1.55844994872371	-2.36672024331388	-1.54624958807773
C	-2.76698661612908	-3.11294339104562	-1.65035709424094
H	-2.75594427918261	-4.04665948026176	-2.21995206999767
C	-3.93341382760316	-2.66702507176163	-1.04771732358835
H	-4.85538654575380	-3.25323927025040	-1.11958441858952
C	-3.93433986013382	-1.42553758592256	-0.35319558177680
C	-5.09178138429885	-0.83937797128951	0.26906528131619
H	-6.03910866944451	-1.38610691914584	0.23280396958466
C	-5.02016016268983	0.38449417188324	0.89564289877440
H	-5.90707210307639	0.81539601731505	1.37016157987940
C	-3.78905660151826	1.12810528047392	0.92881400847574
C	-3.63802811984934	2.40478950257355	1.53436475459106
H	-4.49548916377439	2.88093737454119	2.02095973403509
C	-2.39992780645156	3.04012713753240	1.50083723412719
H	-2.25357669843857	4.01977195930898	1.96285309579601
C	-1.31477800111531	2.41450806204415	0.84863539011854
C	-2.63266428120993	0.56264384506936	0.31796167729176
C	-2.69878846401951	-0.72835212304729	-0.29892701598716
C	1.31478404636407	-2.41188130298080	0.85679405080459
C	2.39992949200252	-3.03528231291458	1.51112369917748
H	2.25358509964667	-4.01336894984396	1.97643121835745
C	3.63801771617480	-2.39981287042607	1.54254121022999
H	4.49547545267021	-2.87430469541677	2.03075703359021
C	3.78903916058869	-1.12517261062247	0.93269768432465
C	5.02013133642831	-0.38165624268380	0.89704705678410
H	5.90703974215283	-0.81093959155781	1.37303704626945
C	5.09174679346731	0.84009537294196	0.26634416024490
H	6.03906596180415	1.38671451265902	0.22825991392162
C	3.93431079320189	1.42413183317123	-0.35792065786570
C	3.93338055562286	2.66326506220012	-1.05663429585203
H	4.85534485882351	3.24924919117722	-1.13045862246234
C	2.76696134359662	3.10712245101823	-1.66081008981403
H	2.75591872275383	4.03890750426870	-2.23355864190132
C	1.55843476395410	2.36123358068253	-1.55421267915038
C	2.69876990793675	0.72711358799817	-0.30132705917243
C	2.63265189923242	-0.56179302269861	0.31991563923865
C	-0.31288806316885	-2.82930631197735	-2.25112291874148
H	-0.50005783193836	-2.88901384618148	-3.33851975038069
H	0.52800297534750	-2.13986994057722	-2.08504153868517
H	-0.01542817430073	-3.84206413169284	-1.92729515760112
C	0.31288367713949	2.82140861275066	-2.26068222582962
H	0.50009453473551	2.87747676481089	-3.34826542283924
H	-0.52798962411638	2.13250277510897	-2.09232259288442
H	0.01537375178607	3.83523543456501	-1.94026311645590
H	-0.33523328295352	2.89800044056876	0.79098047615037
H	0.33524831332175	-2.89558003170773	0.80074070674046

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Bis-mmp triplet

Cu	-0.0000950263147	-0.00072848746600	-0.38330963354598
N	-1.51079381225041	-1.22657706783002	-0.78678814275648
N	-1.42226121556360	1.21138118762096	0.25993778190126
N	1.42218736550193	-1.21067661248074	0.26407165998798
N	1.51081598796264	1.22371585304722	-0.79091014240855
C	-1.53337823018714	-2.38386017207480	-1.49510019740511
C	-2.73898233846523	-3.10215193688198	-1.65962392458995
H	-2.71747542407867	-4.03359820285950	-2.23220173136440
C	-3.93483398981251	-2.64131180152512	-1.09855926918162
H	-4.85986534126033	-3.21630340024059	-1.20808080548292
C	-3.94549049620319	-1.40630141876418	-0.41251803271420
C	-5.11372960957981	-0.79710587124152	0.16885170559664
H	-6.06729054906351	-1.33118195777293	0.10250093753278

C	-5.04633185511347	0.42521164754870	0.79672378619885
H	-5.94361799157810	0.86690695912603	1.24218974022086
C	-3.80978022623727	1.16087663984414	0.87237801723115
C	-3.66416697533827	2.42796857048449	1.48108351251938
H	-4.52875387388009	2.91661818903949	1.94087574728673
C	-2.40226309212931	3.04417108592560	1.48972527527730
H	-2.25456327868752	4.01848882058910	1.96221841111779
C	-1.31394409585211	2.40942404511173	0.87449682171541
C	-2.64655249138656	0.57157764625895	0.29073832997093
C	-2.70467339361015	-0.71292445521527	-0.30856129928020
C	1.31382253510107	-2.40662187711483	0.88269577462054
C	2.40212140606623	-3.03932593519439	1.50006516444800
H	2.25438868632791	-4.01201213701745	1.97587476002266
C	3.66405167157002	-2.42322502629321	1.48930913788922
H	4.52862375359859	-2.91034546744900	1.95074992827834
C	3.80971434011529	-1.15820289053669	0.87632450366997
C	5.04629118472849	-0.42283079700611	0.79818132163047
H	5.94356774114788	-0.86304182104914	1.24513389497872
C	5.11372769335824	0.79736428222683	0.16619054412133
H	6.06731068481818	1.33118963998469	0.09804797155473
C	3.94551026594732	1.40463588695522	-0.41723407118784
C	3.93490115777883	2.63733254300475	-1.10743124685003
H	4.85995580479900	3.21193724650235	-1.21886813586729
C	2.73906951405084	3.09630383457344	-1.67007259427492
H	2.71760232151454	4.02581122843029	-2.24579544533235
C	1.53343963966040	2.37859515408987	-1.50313419011224
C	2.70467116421159	0.71164841495859	-0.31093769698677
C	2.64650682434001	-0.57082831108982	0.29269786490858
C	-0.25053406109596	-2.88233751688858	-2.10957252576694
H	-0.44930700016534	-3.35090703182069	-3.08712178770857
H	0.46813146057982	-2.05938404405579	-2.24886310544956
H	0.23821619905523	-3.64534444367739	-1.476337414441845
C	0.25059724202033	2.87500763236433	-2.11930197575466
H	0.44940384216383	3.34037273656695	-3.09838072753875
H	-0.46802637144576	2.05156865593292	-2.25593221561263
H	-0.23823794844286	3.64007256505483	-1.48861106083728
H	-0.32156798948547	2.86974874331773	0.86200786427818
H	0.32142962412590	-2.86692608701351	0.87178702546990

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Bis-mmp* reduced

Cu	0.04517706882940	-0.01180413338756	-0.22325649694317
N	-1.50939456271279	-0.96586769719975	-1.03127462289947
N	-1.37652869975327	0.93349703803956	0.83265753159593
N	1.46909037189696	-1.05606712491447	0.75606851507822
N	1.59786965388039	0.91471798759689	-1.03253426812029
C	-1.52475610880326	-1.93583997610227	-1.96988490868821
C	-2.74230851633574	-2.52708104194402	-2.39604517260446
H	-2.71257685223726	-3.30857418659192	-3.16122097483580
C	-3.95354997995875	-2.11654944939393	-1.85274747146893
H	-4.89601841655034	-2.56780079563727	-2.18031047437346
C	-3.96306471008658	-1.09999152585902	-0.86199160620109
C	-5.15253763749661	-0.59668074613057	-0.22843385728209
H	-6.12014547312051	-1.01582766452607	-0.52357714704229
C	-5.08533609801953	0.38880529076952	0.72906380263426
H	-5.99891417679534	0.76183496268374	1.20367551648703
C	-3.82278967067827	0.94939970976383	1.13226501732981
C	-3.68014662219266	1.95918275491287	2.11870164465758
H	-4.56794993247121	2.36050445177537	2.61880616382778
C	-2.40611416376870	2.42230705640549	2.43552358444314
H	-2.26336117210782	3.19803885120984	3.19319790380776
C	-1.27724721200917	1.88805640311350	1.77558219842783
C	-2.62954599948139	0.46908863041464	0.51750567245782
C	-2.70218534395479	-0.55900282334646	-0.48556380280695
C	1.38029730648289	-2.05063239838386	1.65427980521046
C	2.50615514059939	-2.64245186173910	2.26443024678041
H	2.36358190615407	-3.45040584764303	2.98734152653148
C	3.78117414716694	-2.18813477334618	1.93572708695199
H	4.67210795119177	-2.63088962685965	2.39326895916190
C	3.92030371450429	-1.13706295722821	0.99309946044685

C	5.18485979289167	-0.58719434194657	0.58134936294822
H	6.10160119726086	-1.00113327432997	1.01409586721732
C	5.24933718353160	0.43610480301610	-0.33571792126150
H	6.21865788799904	0.84478301385118	-0.64006720204265
C	4.05628331714031	0.99118983062751	-0.91749672726119
C	4.04662004709723	2.04448641025331	-1.86869132773837
H	4.99101804667257	2.48620917184761	-2.20363909192962
C	2.83185088654221	2.50117537112060	-2.36613706020897
H	2.80153567087329	3.31068838132788	-3.10166699060525
C	1.61228660925942	1.91969523126333	-1.93392315280766
C	2.79331294104493	0.46447256877616	-0.52953786284842
C	2.72319861980395	-0.60296664657294	0.43120068918069
C	-0.19544014903496	-2.35265533599927	-2.54059242049402
H	-0.16314489444407	-2.20849350600231	-3.63517057297812
H	0.59879748875802	-1.74799949395530	-2.07432140583861
H	0.00930446934058	-3.42060906149861	-2.34603325786943
C	0.27838404341462	2.38197410498965	-2.45697106878271
H	0.21197842746546	2.26640387359476	-3.55346096049409
H	-0.51639456853638	1.78331169172692	-1.98327704642299
H	0.10361414501210	3.44867198468646	-2.22958613586303
H	-0.26142060903133	2.23732344445755	2.00968426096501
H	0.36785766435946	-2.39164679945964	1.89502096777070
O	1.80247418866838	2.79780851295757	2.40569597079449
H	1.98240443365110	3.75474843968994	2.31504133630496
H	2.07456685108786	2.59741231212617	3.32335923470126

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Bis-mmp* oxidized

Cu	-0.02986792560740	0.02396163025315	-0.18119389747683
N	-1.52894974966535	-1.22172531811499	-0.74333980661351
N	-1.53813922189032	1.20251888775637	0.37166024444590
N	1.42439946689703	-1.22034597712859	0.36182386845308
N	1.51115404290880	1.22289884089857	-0.73436074944533
C	-1.49087471738325	-2.36024057102282	-1.46650575194213
C	-2.68272057080933	-3.10926889696011	-1.68604198442291
H	-2.61633982761801	-4.03585156289203	-2.26352702460228
C	-3.90103305095186	-2.67299337672625	-1.18988749323798
H	-4.81109158104082	-3.25980652810744	-1.35193396992667
C	-3.96879993276442	-1.43339860715648	-0.49676320073611
C	-5.18409340560212	-0.84466735892714	-0.00012013959662
H	-6.12247409720219	-1.39227608351109	-0.13156365263252
C	-5.17813435282465	0.38429320697106	0.61962946329279
H	-6.10970085391600	0.82019892083413	0.99336134183052
C	-3.95651144980445	1.12775200648070	0.77492302016632
C	-3.86973396911543	2.41271191916378	1.37487370993576
H	-4.77461772942808	2.89674355032551	1.75664412276931
C	-2.63336835589914	3.04468331578602	1.47048703151754
H	-2.53700496695505	4.03083866772413	1.93191956278286
C	-1.48247894905387	2.40757742962597	0.95603170306095
C	-2.74218242909051	0.55564155530821	0.29670105315544
C	-2.74296649631776	-0.73887299595025	-0.31689405216355
C	1.31935629835482	-2.41708654984481	0.95376461096621
C	2.43934437020439	-3.09524172816430	1.48313873159306
H	2.30084903181313	-4.07086742720658	1.95602585394227
C	3.70042455548670	-2.51588964748175	1.37973684256069
H	4.58497362010658	-3.03308742700562	1.76561452387066
C	3.84020755024079	-1.24211285492108	0.76558928054696
C	5.09362428557532	-0.55586749310766	0.60106251157386
H	6.00680895730388	-1.03311042578609	0.96972003191773
C	5.15085444064703	0.67053412327899	-0.02106569463978
H	6.11234274855959	1.17458435685648	-0.16019527473616
C	3.95970089041811	1.31563118997119	-0.50672672370333
C	3.94640664455946	2.56366219814754	-1.18862700606496
H	4.88306540540571	3.10571070891155	-1.35514399090651
C	2.74573703539379	3.06702454519524	-1.66228624594636
H	2.71784977393677	4.00493371138406	-2.22438965409756
C	1.52126933310192	2.37408686133905	-1.43521898932596
C	2.70384229946586	0.67708209966273	-0.32370818522678
C	2.65034960599910	-0.61926939131893	0.28736825917832
C	-0.19499519393134	-2.81626206675916	-2.08085179426272

H	-0.34678651445788	-3.02194253481198	-3.15484350113702
H	0.59171095230557	-2.05519689390508	-1.98171686127289
H	0.16197900003698	-3.75863777827385	-1.62801722885097
C	0.23889596135942	2.91186014216856	-2.00960400940267
H	0.36801601953728	3.11219160302052	-3.08769739149349
H	-0.59198669375207	2.20281246260169	-1.88651082216958
H	-0.04071358207347	3.87361237263723	-1.54323834170044
H	-0.49409204909759	2.86529978497266	1.02885466478393
H	0.31803873308101	-2.85541720715097	1.00109217782353
O	0.76082692790521	0.99929304873034	2.39960204175233
H	1.61722919783853	1.32261780465683	2.74578904848556
H	0.24889708080953	0.80475245157281	3.21107477032801

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Bis-mmp* triplet

Cu	-0.03430337382588	-0.02976425301839	-0.16671717988840
N	-1.52613404335493	-1.26096229184441	-0.7263362709475
N	-1.50843845185713	1.15338384095346	0.37485906369963
N	1.40179525047455	-1.27169297482241	0.33462164264162
N	1.48468705744642	1.18636006464546	-0.68281228711499
C	-1.50631714563923	-2.39260018509605	-1.47617515464393
C	-2.70163715738800	-3.09415269229547	-1.75452530633299
H	-2.64215182531698	-4.00743907078684	-2.35307224061652
C	-3.93415284239497	-2.63882925190184	-1.27675016680555
H	-4.85259161364968	-3.20004570812718	-1.47629088218337
C	-3.98809656548468	-1.42003374388206	-0.56449570946972
C	-5.19695622749557	-0.80735752309008	-0.07765753698490
H	-6.14594773611800	-1.32969998235860	-0.23729743079272
C	-5.17373420432425	0.40601944964385	0.56992404369167
H	-6.10266184646786	0.85356958184734	0.93811703055866
C	-3.94098814225388	1.12545132333677	0.76390326420494
C	-3.83766473757216	2.38701114125696	1.39301679171741
H	-4.73619320085049	2.88341053975651	1.77285000667949
C	-2.57503488700841	2.98538459779962	1.52614313804875
H	-2.46070167872300	3.95356925512441	2.02050343320520
C	-1.43923428203317	2.34098926434397	1.01231511176221
C	-2.73574717887683	0.52862832079832	0.28396771265727
C	-2.75194732748075	-0.74700248186380	-0.33860425883830
C	1.30232160460300	-2.47567767661066	0.93813645332802
C	2.41280467322076	-3.15259301632653	1.46096773907145
H	2.27181764594281	-4.13139113645373	1.92660434014388
C	3.68946074461677	-2.57267055330849	1.36691771833462
H	4.57186093159422	-3.09467970290074	1.74981008373287
C	3.82613161639741	-1.29865396102611	0.76958002836374
C	5.07639781668001	-0.59915252251950	0.61347692121709
H	5.99051552113976	-1.07706481226465	0.98079856264926
C	5.13480656702432	0.63176355736214	0.00168157296057
H	6.09721192866071	1.13737210486816	-0.12962328201043
C	3.94632088176508	1.28534326818210	-0.48149756092792
C	3.92819130565292	2.52967391519083	-1.14931235280943
H	4.86188655337827	3.07587471783947	-1.31788727754357
C	2.71197568311670	3.03422433480016	-1.61904758800492
H	2.67932117092331	3.97365568967209	-2.17772207688163
C	1.49849826628440	2.34839195321010	-1.37886718930853
C	2.69231291796621	0.63050124328783	-0.29556629922923
C	2.64089206515226	-0.66366240758967	0.28651709852541
C	-0.19190629173631	-2.88390788772058	-2.02562493367235
H	-0.34858065820306	-3.39866878637656	-2.98713238085892
H	0.50981601860240	-2.04866990497870	-2.17783812958491
H	0.29800695218827	-3.60397706551239	-1.34472644111206
C	0.19692138190437	2.89778846298476	-1.90353171433903
H	0.36460502030800	3.45635963815715	-2.83833093664156
H	-0.52591413048749	2.08921355807555	-2.09638508539932
H	-0.27257440660343	3.59441873747585	-1.18507820433893
H	-0.43862341018684	2.76375868954668	1.12577069749291
O	0.29753071454721	-2.90580728630561	0.99220453572901
H	0.82611459694409	0.96097744891589	2.47720984844282
H	0.36254948806658	0.78259344584463	3.31964201021308
H	1.77246016073216	0.94316930906099	2.72234927035727

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Bis-dmp reduced

Cu	-0.00000001556824	0.00000202908429	-0.00006690130349
N	-1.50591262753092	-0.94569530113254	-0.94239339292400
N	-1.50585600257644	0.94575690048616	0.94240624338822
N	1.50585378316701	-0.94243861174716	0.94572599457920
N	1.50591475478440	0.94237962350462	-0.94570775255642
C	-1.45942139085072	-1.90106459179680	-1.89423635022500
C	-2.64703481883459	-2.45210599331966	-2.44309233454743
H	-2.56584549739128	-3.22510256811107	-3.21315501180185
C	-3.89218917971325	-2.01661054100575	-2.00913337418290
H	-4.81118834698924	-2.43854189668620	-2.42939101720778
C	-3.96846020254001	-1.01236435521252	-1.00865369038064
C	-5.20035399862990	-0.48726374940255	-0.48547511747828
H	-6.14502305723745	-0.87947418287108	-0.87621500873085
C	-5.20032461725901	0.48743750344605	0.48560151116665
H	-6.14497007626413	0.87967670395259	0.87636967045674
C	-3.96839892214250	1.01249997672068	1.00874264813786
C	-3.89206566235463	2.01674565724047	2.00921826181389
H	-4.81103893432897	2.43870841322924	2.42950127153710
C	-2.64688508096443	2.45220136483827	2.44314064315350
H	-2.56564788593789	3.22519599032697	3.21320029817653
C	-1.45930529428340	1.90111824939664	1.89425005766710
C	-2.73394022697632	0.50956015790717	0.50770305050072
C	-2.73397203822355	-0.50946134890787	-0.50765125537001
C	1.45930083583521	-1.89428836223411	1.90108127095636
C	2.64687936593742	-2.44319446984003	2.45215170776232
H	2.56564041651698	-3.21326410473477	3.22513621960951
C	3.89206093244233	-2.00927178727437	2.01669911864333
H	4.81103326458960	-2.42956632709530	2.43865245415324
C	3.96839651034207	-1.00878104964515	1.01246867401840
C	5.20032342015237	-0.48563537026068	0.48741358054015
H	6.14496796018605	-0.87641054895842	0.87964800092934
C	5.20035508037745	0.48545444685896	-0.48727452496703
H	6.14502505530329	0.87619823981375	-0.87947884611050
C	3.96846250042718	1.00864148815463	-1.01236953710314
C	3.89219384133130	2.00913259275462	-2.01660450311573
H	4.81119399362703	2.42939307040382	-2.43853087826211
C	2.64704049177927	2.44309811626396	-2.45209630908232
H	2.56585298762360	3.21316962150420	-3.22508428071151
C	1.45942578110202	1.89423713930815	-1.90106271955156
C	2.73397317875933	0.50763332216641	-0.50947509550189
C	2.73393895541839	-0.50773262308307	0.50953481967502
C	0.09801804300783	-2.34819484478556	2.35651985829442
H	-0.04304301922241	-2.17109438966440	3.43770165543878
H	-0.67471101556707	-1.79465940433331	1.80077261058807
H	-0.04285271086274	-3.43006336400595	2.18352567797595
C	-0.09802354595793	2.35654129258811	2.34817519324243
H	0.04288013333724	2.18340273169129	3.43001744198611
H	0.67470673568450	1.80088050698537	1.79455464165227
H	0.04300257978877	3.43775020591253	2.17121930795157
C	-0.09816656609832	-2.35654158438772	-2.34818685105123
H	0.04268079085441	-2.18353457093364	-3.43005652007591
H	0.67459330466083	-1.80082239072250	-1.79466497911628
H	0.04286782301292	-3.43772964568207	-2.17110503758227
C	0.09817201019103	2.34820115245404	-2.35652936267475
H	-0.04283007696704	2.17123588511798	-3.43774000563434
H	-0.67458906864327	1.79460662120025	-1.80088421556585
H	-0.04270565032417	3.43004897452304	-2.18340601117970

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Bis-dmp oxidized

Cu	0.00000005897389	0.00004253193076	0.00000124663207
N	-1.49267324296994	1.13597812056448	-0.71810133596153
N	-1.49259488022790	-1.13592967549953	0.71820405314176
N	1.49259355986948	-1.13593102105601	-0.71820224296058
N	1.49267442234323	1.13597690088414	0.71810327658094
C	-1.43078752600779	2.21791424420801	-1.52099247148275
C	-2.62660006027911	2.83123767806096	-1.99098241935158
H	-2.54400510308673	3.70746075836244	-2.64031270886464

C	-3.86832292230036	2.33536158793773	-1.62686183702479
H	-4.78581426932300	2.82190279873981	-1.97383972091110
C	-3.94903048452227	1.17618906685272	-0.80657747102017
C	-5.18167212521131	0.56413970353621	-0.39447881367673
H	-6.12533047945400	1.01406725369833	-0.71796766817540
C	-5.18163180327773	-0.56428554647679	0.39468477700144
H	-6.12525773907642	-1.01426345513147	0.71819812792173
C	-3.94894670190354	-1.17626854137919	0.80675135532412
C	-3.86815436671818	-2.33543632424302	1.62703402767861
H	-4.78561019322147	-2.82202665298198	1.97403699196972
C	-2.62639495815297	-2.83124601954443	1.99112058516070
H	-2.54373579921576	-3.70746409838721	2.64044958001309
C	-1.43062791209024	-2.21786097782186	1.52109492871075
C	-2.71634702634146	-0.59924069717883	0.39305973347597
C	-2.71638877376992	0.59922777973229	-0.39291824277149
C	1.43062546189426	-2.21786241307919	-1.52109284988270
C	2.62639180807987	-2.83124859892578	-1.99111890989756
H	2.54373156407183	-3.70746696750503	-2.64044739367454
C	3.86815174780711	-2.33543939981392	-1.62703359815938
H	4.78560703977157	-2.82203042347703	-1.97403699923385
C	3.94894532197934	-1.17627113454135	-0.80675165886028
C	5.18163111526456	-0.56428838447708	-0.39468673039348
H	6.12525652924753	-1.01426681675773	-0.71820085649956
C	5.18167274005945	0.56413734993132	0.39447616998838
H	6.12533159853009	1.01406485443192	0.71796363560840
C	3.94903181068789	1.17618719807413	0.80657598898024
C	3.86832579759666	2.33536026149851	1.62685975946236
H	4.78581781707102	2.82190155530099	1.97383574127896
C	2.62660362883199	2.83123667487892	1.99098203624689
H	2.54400977334970	3.70746008501082	2.64031203298369
C	1.43079023154777	2.21791284917517	1.52099468882157
C	2.71638940269895	0.59922610695686	0.39291860398173
C	2.71634629713772	-0.59924255418552	-0.39305910778230
C	0.09061349605190	-2.76687344879416	-1.92609373652346
H	-0.07242732372565	-3.77300503552404	-1.49953950189005
H	-0.73098676190832	-2.11083425599234	-1.60521989290970
H	0.04133391352888	-2.87816592856275	-3.02336765433142
C	-0.09061636642869	-2.76687360816945	1.92609514708812
H	0.07242811180064	-3.77300018627479	1.49953034097704
H	0.73098365007951	-2.11082937393440	1.60523085878251
H	-0.04134030866312	-2.87817794843197	3.02336792621068
C	-0.09081612503957	2.76699782644124	-1.92602912715064
H	0.07220476305122	3.77311471524158	-1.49943174994837
H	0.73082387626039	2.11097534302055	-1.60522180144109
H	-0.04158956781404	2.87834760512141	-3.02329917612142
C	0.09081986138295	2.76699475821882	1.92603683936406
H	-0.07219360302252	3.77312213282280	1.49946167487566
H	-0.73082226096695	2.11098350844272	1.60521216429954
H	0.04158928574956	2.87832023907121	3.02330938433979

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Bis-dmp triplet

Cu	0.00004463812313	-0.00038761761802	-0.00045994924741
N	-1.47250519093404	-1.15803482324761	-0.66228209932747
N	-1.47231847320447	1.15764329816723	0.66151826178691
N	1.47232237252630	-1.15586300274203	0.66597665006641
N	1.47255212025706	1.15503031763566	-0.66610521883810
C	-1.41293809569936	-2.25124214539501	-1.46652598930436
C	-2.59518111955667	-2.86748089478761	-1.92970027725412
H	-2.50899763522013	-3.75012327105492	-2.56932604305127
C	-3.85394467211012	-2.36990988851013	-1.57241924908069
H	-4.76755440047526	-2.86716411265657	-1.91330890572390
C	-3.93747087817895	-1.20083577833839	-0.78358596123400
C	-5.16851011119822	-0.57216734344200	-0.38166162904431
H	-6.11333860153576	-1.02877764582933	-0.69400130407628
C	-5.16837594002403	0.57091588463675	0.38354019042356
H	-6.11309366792395	1.02738315750348	0.69642432004528
C	-3.93720810965215	1.19994233232591	0.78449942751803
C	-3.85341227637500	2.36930841636248	1.57287367701498
H	-4.76690037271740	2.86652907547492	1.91413987788406

C	-2.59451073222010	2.86754298391488	1.92873915989190
H	-2.50807423762115	3.75072768937362	2.56758129759394
C	-1.41245645262482	2.25142601820396	1.46490317369911
C	-2.70817188367637	0.60504874421686	0.37099398149674
C	-2.70829461840668	-0.60580965561571	-0.37069616959560
C	1.41250334938724	-2.24615333832771	1.47415289023262
C	2.59459601951036	-2.86056114693554	1.94013532116433
H	2.50820756766775	-3.74093540583317	2.58285191252934
C	3.85348216861905	-2.36410753270872	1.58173057760190
H	4.76697601193435	-2.86001684235279	1.92488264465570
C	3.93725562252436	-1.19787102878218	0.78874137818784
C	5.16840943489061	-0.57046684320860	0.38518144178328
H	6.11314249464692	-1.02579753135244	0.69967134787256
C	5.16851989949837	0.56982040308641	-0.38418131052356
H	6.11334055410893	1.02527558964452	-0.69822672699734
C	3.93747192207886	1.19721962603341	-0.78805259739005
C	3.85387602689381	2.36374267709303	-1.58065469673384
H	4.76745317848181	2.85988656336698	-1.92324786210184
C	2.59507426004294	2.86051666377659	-1.93892899988356
H	2.50882803408834	3.74139379876543	-2.58097627058861
C	1.41289144900900	2.24589485517947	-1.47344944817994
C	2.70832598571112	0.60363679253938	-0.37300266928710
C	2.70820431453111	-0.60454596552082	0.37303039361688
C	0.05641433933191	-2.77445694440955	1.86719407343430
H	0.11931708397461	-3.34505827225853	2.80696275884491
H	-0.66214595076943	-1.94909160975466	2.00118629744319
H	-0.36328080893098	-3.44827533745271	1.09853885374197
C	-0.05631351368264	2.78219398413505	1.85439216713340
H	-0.11871730687086	3.35700599457787	2.79162250983154
H	0.66281218000955	1.95782614998267	1.99151463231051
H	0.36235038860044	3.45276645163794	1.08231451065364
C	-0.05695994398679	-2.78078982180314	-1.85829664647128
H	-0.12012427854408	-3.35425352826055	-2.79630683702983
H	0.66160627558837	-1.95587036532327	-1.99500232380785
H	0.36290390259655	-3.45229138888526	-1.08771212184573
C	0.05680668023282	2.77498664390231	-1.86541260831139
H	0.11921594567824	3.34534117180979	-2.80536642575551
H	-0.66240046332636	1.95004798542220	-1.99850505136520
H	-0.36170548507817	3.44928581363824	-1.09648733640869

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Bis-dmp* reduced

Cu	0.02661606051486	-0.01134278484476	-0.03381311428640
N	-1.49279912204091	-0.94016188645350	-0.95738974008517
N	-1.46413652102839	0.94763580015806	0.93023404362597
N	1.57138670396573	-0.93704624768167	0.85070533016873
N	1.49176060162452	1.02935108993739	-0.95322904014510
C	-1.45899608171669	-1.91023768381466	-1.89524984186707
C	-2.65591801343890	-2.42488333483068	-2.46070282815910
H	-2.58558759873764	-3.20376133447537	-3.22587118052249
C	-3.89374168007881	-1.94737944705432	-2.05089515266803
H	-4.81883160460033	-2.33906921173014	-2.48709851488728
C	-3.95518644876315	-0.93924557858498	-1.05328737821124
C	-5.17815087532136	-0.37641772868643	-0.54901775204324
H	-6.12826344015107	-0.74107836171321	-0.95328064877243
C	-5.16362600711397	0.59892870309000	0.42143725463066
H	-6.10170785374252	1.01883857827095	0.79912286833126
C	-3.92422634700682	1.08674888622563	0.96225737705874
C	-3.83222166902790	2.08449922857701	1.96790192294698
H	-4.74445964135590	2.53162946058967	2.37680686641966
C	-2.58118601734216	2.47994622105060	2.42268308200376
H	-2.48769716904435	3.24497367444085	3.19935827186458
C	-1.40290965397200	1.89575560997144	1.88790175881771
C	-2.69825031021031	0.54885981180463	0.47685419484797
C	-2.71350213691126	-0.47041029296148	-0.53783655827090
C	1.56377307599455	-1.94800995624525	1.74504391672323
C	2.77382509508543	-2.45164742906346	2.29200307046884
H	2.72454604174391	-3.26458883005961	3.02258568613392
C	3.99816063275624	-1.92104607063351	1.90754325990301
H	4.93338574847079	-2.30409220157391	2.32958133692289

C	4.03244235702570	-0.86939264864384	0.95463448471123
C	5.23963837331523	-0.25020062869503	0.47915163432213
H	6.19915544889166	-0.60448067343464	0.87021354271630
C	5.19877415340297	0.76542617861719	-0.44824167381166
H	6.12499949695385	1.22817661042912	-0.80453673501476
C	3.94685801801751	1.24040604064969	-0.97146383493098
C	3.82812020472849	2.27781004537730	-1.93322888314839
H	4.72792008831378	2.76824049536288	-2.31941477039286
C	2.56704297569648	2.65646657105517	-2.37437916283141
H	2.45273014362824	3.45142925785990	-3.11748237888271
C	1.40511584575389	2.01595853849503	-1.86911513506390
C	2.73597812726396	0.64697147872017	-0.51372267712728
C	2.77875633708419	-0.41454396033813	0.45592304802620
C	0.22973560507975	-2.53854319461523	2.10637761964259
H	0.16205269561340	-2.76775087934672	3.18326528592729
H	-0.57138910272221	-1.83514225500165	1.82802973233107
H	0.07137535452033	-3.48004158525191	1.54294858985518
C	-0.03561505842137	2.30576423259535	2.36679182517208
H	0.08199534672115	2.11876498346254	3.44916352454754
H	0.72887989757880	1.73146151277149	1.82134625707784
H	0.14144725037470	3.38358818346554	2.20197845085067
C	-0.10966902708052	-2.44363968227246	-2.28765024687600
H	-0.03119272480212	-2.59420648634992	-3.37772011050722
H	0.67242476866339	-1.74253171764547	-1.95493445710388
H	0.06789540508321	-3.41870969393291	-1.79156354170430
C	0.02745997544081	2.40663618394819	-2.33437314399688
H	-0.08403962084035	2.25828862749151	-3.42338474662348
H	-0.72145258151411	1.79084076739920	-1.81307231973471
H	-0.17929701413975	3.47202680695136	-2.12856352048697
O	0.09217774679549	-5.13071975520233	-0.14820261825751
H	0.86963508966543	-5.72346722686265	-0.17465429783234
H	-0.66874711564359	-5.74462433676802	-0.12376797080238

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Bis-dmp* oxidized

Cu	-0.05889220177200	0.04090030881626	0.03102008588939
N	-1.49917885049449	1.17832287337042	-0.84002092836201
N	-1.59571335293777	-1.06167703324255	0.63124085810075
N	1.41875689657004	-1.13575735423685	-0.71659717107747
N	1.44952921637304	1.17049304134321	0.65203601054182
C	-1.38317897238937	2.25234836971001	-1.64897234994748
C	-2.53701819144073	2.81833583442940	-2.26018477169686
H	-2.41020208363448	3.68920660097178	-2.90924059520931
C	-3.79637974172641	2.28575298035876	-2.03154301675022
H	-4.68298375701112	2.73640631263431	-2.48952392939324
C	-3.93204464450740	1.13708614729322	-1.20599518087379
C	-5.18373319186124	0.49042197081208	-0.92087226811053
H	-6.09844589709404	0.90286659907944	-1.35765678472155
C	-5.23820930632831	-0.62043939152972	-0.10974410111083
H	-6.19808167203089	-1.09482810910817	0.11658293734182
C	-4.04130866635144	-1.18072671322494	0.45512893578912
C	-4.01294161215207	-2.31350869511433	1.31367609987306
H	-4.94585524101609	-2.82784865630870	1.56706518333453
C	-2.80401552292882	-2.75015898894269	1.83532800728166
H	-2.76777776024613	-3.60282121880111	2.51882264877738
C	-1.58419485767123	-2.10534919485148	1.48720690977108
C	-2.78914582556359	-0.57407411318833	0.16101160875658
C	-2.73509888625851	0.60808109718688	-0.64780996180281
C	1.33925051041208	-2.24598237385875	-1.47974676627312
C	2.51977864507919	-2.83951396297623	-2.00833688043763
H	2.42221886112272	-3.73945751727940	-2.62180989760373
C	3.76790026743980	-2.29679888145544	-1.74457883068762
H	4.67443939141102	-2.76795279512796	-2.13840183151384
C	3.86634393575584	-1.11123800033803	-0.96733768787091
C	5.10433440017235	-0.45200264913929	-0.65284652328996
H	6.03794836667737	-0.88409947699287	-1.02601343035312
C	5.12240448507951	0.69509337601775	0.10794784557487
H	6.07136118895285	1.17949882263589	0.35785145406367
C	3.90107973981897	1.28079568125031	0.58838079277104
C	3.83421365839326	2.45215390264790	1.39129565147333

H	4.75515911663138	2.97743517710194	1.66519869499221
C	2.60274762882605	2.91274184624544	1.83340025354823
H	2.53573300563925	3.79617852952681	2.47415470932873
C	1.39948372165015	2.25280619341359	1.45699172532091
C	2.66307058091403	0.66114411701032	0.26302131931103
C	2.64524801891414	-0.55718354394489	-0.49183188142106
C	-0.00678237579897	-2.85710892102096	-1.75917445642970
H	-0.24348743617660	-3.64525731337248	-1.02052479378121
H	-0.80713809713617	-2.10320960465218	-1.72245441219630
H	-0.01599759470561	-3.33325406385065	-2.75256589956353
C	-0.28042931001062	-2.51420080994670	2.10806966334611
H	0.56177198082948	-2.40084619162611	1.40683269337146
H	-0.08609235565731	-1.84991946182349	2.97646234687743
H	-0.31148395699145	-3.55410772930983	2.46749069984189
C	-0.02524123851456	2.85268106514070	-1.89163897706790
H	0.17530092321260	3.67556763977231	-1.18068898919317
H	0.77242091705581	2.10324880304282	-1.78037097230338
H	0.03217542377230	3.28116668715076	-2.90492387154436
C	0.06851595680130	2.69060845961620	1.99467072002620
H	-0.74029422730734	2.53847581015221	1.26218631942011
H	-0.16568733503319	2.07184597359321	2.88650592228383
H	0.08258087279018	3.74792647412109	2.30039538844272
O	-0.15487638228984	0.13962204426487	4.19673332334869
H	0.59825609237837	0.14171525720224	4.82290908181461
H	-0.93702132963532	0.16422814835204	4.78576001997239

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Bis-dmp* triplet

Cu	-0.03008670372458	-0.01948153265282	-0.05883466116568
N	-1.53198632412941	-1.16867270161531	-0.62353527531882
N	-1.47654905596326	1.16055360663956	0.67521427196073
N	1.41534346543968	-1.18269932693429	0.70265372526629
N	1.47294914741892	1.11594774663392	-0.64958456681870
C	-1.50766402384499	-2.26613358428110	-1.42153981389641
C	-2.70706081756109	-2.92917935613502	-1.76294345102856
H	-2.64985027289164	-3.82253296164421	-2.39069693407647
C	-3.94400348650273	-2.46066529329620	-1.30404545062511
H	-4.86820474714962	-2.99388809790686	-1.54919100139101
C	-3.99397872426471	-1.28146257863454	-0.52887676011999
C	-5.20226248551533	-0.68591064211303	-0.02250769475349
H	-6.15733145557227	-1.17346028065790	-0.24400359485492
C	-5.16650882327681	0.46291994875797	0.73253671048142
H	-6.09212105942444	0.89496812371155	1.12685724113813
C	-3.92355766674723	1.13103775464551	1.01856216596761
C	-3.80793759165466	2.30719300406389	1.79128971387137
H	-4.70242230758394	2.77814667327244	2.21110160747466
C	-2.53849687716563	2.84828721554009	2.02663997255462
H	-2.42322178229018	3.74310703858016	2.64428883234366
C	-1.38406080546269	2.26643659528516	1.46180109019128
C	-2.71764418575576	0.57095924291345	0.49986544195593
C	-2.75107498588457	-0.64510218493891	-0.23250727331652
C	1.32176839061994	-2.26996772965827	1.51470630854357
C	2.47567162450299	-2.83969444401965	2.09282191083950
H	2.35957414017712	-3.71983715924050	2.73106343555042
C	3.74560425074882	-2.30537244401926	1.84506707592500
H	4.63966513177876	-2.76723186543634	2.27573938534954
C	3.86231197113826	-1.14749323744547	1.04533240231775
C	5.10589592711733	-0.48723003037273	0.74417572196973
H	6.03106656055099	-0.91086614955061	1.14853051828616
C	5.14273567461491	0.64386520816429	-0.03710956557581
H	6.09820086041956	1.12546971587781	-0.26963328228363
C	3.93503774352904	1.22858336338639	-0.55725367538594
C	3.88618345749625	2.38973416960340	-1.35929383181402
H	4.81081869164429	2.91649502491859	-1.61649878167664
C	2.64977392658755	2.84870635729442	-1.82897138155256
H	2.59351004267345	3.72749586171917	-2.47704311483018
C	1.44969859511996	2.19473639107136	-1.47255620295887
C	2.69149061752803	0.60025052174790	-0.24668389354236
C	2.65695912933779	-0.59854210233024	0.51367955888732
C	-0.04049939106132	-2.85575151974983	1.77993814406317

H	-0.01450778675466	-3.51518062320764	2.66115612882677
H	-0.78407090197166	-2.06038717144300	1.95523569690983
H	-0.40250823144099	-3.45394091069657	0.92406092023103
C	-0.02233356318104	2.85958796668092	1.71306123283789
H	-0.04893844199460	3.53996702246809	2.57818423682401
H	0.72192566442393	2.06930116217504	1.90741071682528
H	0.33915696861935	3.43736278664145	0.84306061467454
C	-0.18288722315499	-2.70948722935795	-1.98206102805602
H	-0.24960438655663	-3.72699798826624	-2.39792095966524
H	0.10767225598548	-2.01661546108092	-2.79746466877600
H	0.61715187789383	-2.68714046120410	-1.22559747877059
C	0.12546323379806	2.62624784497503	-2.04340424211598
H	0.19186155325760	3.63562592886840	-2.47870256538282
H	-0.16301205079038	1.91754729583006	-2.84582561666617
H	-0.67563561305634	2.61748508108632	-1.28780655645656
O	-0.02561038385500	-0.06507477244907	-4.12979565517565
H	-0.79223829729523	-0.15196757792686	-4.73146524097685
H	0.73936387705647	0.00384421671314	-4.73588379703960

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Bis-dbp reduced

Cu	0.00341217715995	0.00210817677988	0.00853837900580
N	-1.49764349217161	0.57497602788224	-1.20922268074436
N	-1.51189349460932	-0.53769984517958	1.21897297825727
N	1.49658014079380	-1.23185962609714	-0.54922291736321
N	1.52645664371129	1.19645314385988	0.56274721324221
C	-1.44240868247405	1.13670203899103	-2.43542610826328
C	-2.62668853640842	1.48951933940252	-3.13525761121136
H	-2.53988282447188	1.95235008828587	-4.12296670569629
C	-3.87515708771162	1.25148976185702	-2.57536773670397
H	-4.79139033601142	1.52232641820546	-3.11071718597538
C	-3.95905582815141	0.64997818079210	-1.29216482097720
C	-5.19496434160307	0.35163593217800	-0.62068888371793
H	-6.13645268570301	0.59765542597566	-1.12283581849574
C	-5.20235281549466	-0.23208883622586	0.62533359046883
H	-6.14980099089942	-0.45706417948296	1.12614179950573
C	-3.97433785719338	-0.55791838646926	1.29845061025341
C	-3.90555357126687	-1.16142140207125	2.58154273847985
H	-4.82827696925473	-1.41197255830569	3.11562235151339
C	-2.66349432288792	-1.42751224205732	3.14309999001370
H	-2.58859544922124	-1.89216920994678	4.13092869835903
C	-1.47069630384026	-1.10114838247096	2.44518603311030
C	-2.73596509758288	-0.26927544944874	0.65692923571681
C	-2.72824482070738	0.33409509940918	-0.64894297484967
C	1.43323939003165	-2.45732658306105	-1.11175594369350
C	2.61318179566908	-3.17259487144229	-1.44765984964371
H	2.52001842714070	-4.15930229096162	-1.91135659342883
C	3.86535038940555	-2.62890286996083	-1.19214176865265
H	4.77825214228803	-3.17634340702839	-1.44975500678068
C	3.95743635797565	-1.34647599764857	-0.59020930732162
C	5.19761090164503	-0.69059242834599	-0.27538524874047
H	6.13587258169547	-1.20514026852017	-0.50773128587803
C	5.21297904382648	0.55602478138806	0.30685570834603
H	6.16363366513170	1.04494991517916	0.54411849171242
C	3.98933532202408	1.24530243829032	0.61496804716862
C	3.92870810378772	2.53035427161746	1.21503828288214
H	4.85463198787727	3.05339322178988	1.47679893171223
C	2.69035564815931	3.10805168935286	1.46342017458577
H	2.62206953989994	4.09795277368903	1.92469844241729
C	1.49327126609863	2.42434708223069	1.12322660071322
C	2.74687360264521	0.61896166371071	0.31082027881193
C	2.73075409991849	-0.68729101203385	-0.29167640373871
C	0.06199854912488	-3.04304539974444	-1.34284924029443
H	-0.67396606018452	-2.24053113204836	-1.15587769099201
H	-0.03868996577887	-3.34776933044499	-2.40289067072807
C	0.13702635393865	3.04660018575231	1.34670363741437
H	-0.61875703473540	2.26265080816980	1.15934054518820
H	0.03971839518351	3.35766684204455	2.40517257396158
C	-0.10969171939929	-1.34316654331416	3.05001752972982
H	0.63861711853063	-1.16144089420531	2.25770999245060

H	-0.02101039791928	-2.40394089045805	3.35575243936072
C	-0.07591740852221	1.34713495658986	-3.03951171403362
H	0.66764859263080	1.15718765654987	-2.24470739658004
H	0.03403402815723	2.40335166615040	-3.35400512030275
C	-0.13749562993780	4.26711853012820	0.43570314522403
H	-0.05382782307909	3.95252927558071	-0.62282011064291
H	0.64670951986478	5.03311264825610	0.59312779923419
C	-1.52119068784245	4.89051076307908	0.68587575690495
H	-1.59659631060170	5.19137571226687	1.74917079475506
H	-2.30080192805411	4.11937124024599	0.52915469199284
C	-1.80246302336427	6.10269745510249	-0.21415667861442
H	-1.76830552844235	5.82645350942035	-1.28354395458781
H	-2.79976616573732	6.52816174708300	-0.00996432310390
H	-1.05834457989352	6.90307595496513	-0.05307880218973
C	0.18971423056207	-0.44059233143976	4.27103417606198
H	0.11506664381100	0.62015487001989	3.96181860840756
H	-0.58760682521148	-0.59199781545450	5.04523533668328
C	1.57731792716420	-0.70974067010778	4.87761974489302
H	1.64345341367878	-1.77512354839483	5.17321266107915
H	2.34982157533166	-0.55899486607550	4.09818585363327
C	1.88305579521518	0.18180036504642	6.09010936943990
H	2.88219844300758	-0.03678715421566	6.50396289743583
H	1.85959841265857	1.25264291558459	5.81845835105255
H	1.14561964978607	0.02692282792009	6.89787590347746
C	0.20744166035424	0.42847206566370	-4.25246087920089
H	0.11528888908239	-0.62794802567699	-3.93324698674420
H	-0.56801231424489	0.58575795647545	-5.02734942384318
C	1.59879620562097	0.66893593578970	-4.86241198798225
H	1.68161406450324	1.72981322648385	-5.16976340605490
H	2.36943310133002	0.51455021675674	-4.08184067232099
C	1.88952533980881	-0.24033540470445	-6.06542657434506
H	2.89198117897813	-0.04257193151602	-6.48173682834171
H	1.84866718788854	-1.30776500384168	-5.78258871824179
H	1.15441202811268	-0.08194819875649	-6.87463233933552
C	-0.24722609144196	-4.26016382986239	-0.43827247928343
H	-0.16077218563929	-3.95243200280704	0.62202647680997
H	0.51876693933759	-5.04443166253216	-0.59552251968800
C	-1.64456991636863	-4.84823007069145	-0.69787832657745
H	-2.40571499417771	-4.05870818928465	-0.54208089626736
H	-1.72171018647253	-5.14287759661277	-1.76278997029962
C	-1.96033795715959	-6.05667183092889	0.19564584150982
H	-1.92614539507927	-5.78554612994022	1.26633420189634
H	-2.96627356038351	-6.45735009315863	-0.01624919421192
H	-1.23467627321166	-6.87410540901670	0.03583085181209

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93

Bis-dbp oxidized

Cu	-0.00021591958251	-0.01481233141727	-0.00004070177213
N	-1.19022021264497	-1.50900080248587	-0.62228445452488
N	1.19079489213763	-1.50835739492167	0.62060373149177
N	1.02137484959566	1.48016500786823	-0.87184694442905
N	-1.02344738173351	1.47899232452682	0.87097980145696
C	-2.33936237447818	-1.44429273419531	-1.32678394845714
C	-2.99724136615692	-2.64227863080212	-1.72949970540527
H	-3.93265090938511	-2.55926557102613	-2.29013817743526
C	-2.47326816956203	-3.88403136813125	-1.40861553699159
H	-2.99430162616600	-4.80183470315116	-1.70060931216110
C	-1.24232260096503	-3.96508585169373	-0.70030208675186
C	-0.59570908259043	-5.19731114008253	-0.34402351211126
H	-1.07313700002993	-6.14123197142503	-0.62473267794415
C	0.60041758389867	-5.19699556412643	0.33865492783359
H	1.07886465027199	-6.14066444601886	0.61847282841011
C	1.24572752431012	-3.96440568360386	0.69601760234439
C	2.47678667562364	-3.88265281142371	1.40407204913421
H	2.99895078058094	-4.80016223202973	1.69496842807337
C	2.99942463111678	-2.64063457987609	1.72615974367141
H	3.93486497137667	-2.55714834576903	2.28667381022747
C	2.33989678380593	-1.44301403736975	1.32511442442225
C	0.63126332588573	-2.73212911103390	0.33933604354517
C	-0.62926885554533	-2.73245573902502	-0.34239504707231

C	1.96264194676384	1.41336730526222	-1.83736993083050
C	2.47289825230188	2.61031070549057	-2.41714116005366
H	3.22653728806847	2.53025444155218	-3.20504702937599
C	2.03411164362430	3.85259967802376	-1.98843209210090
H	2.44709341622629	4.76937108566625	-2.42214531041628
C	1.02777745737356	3.93558280352554	-0.98696964640589
C	0.48758249743067	5.16789879888335	-0.48355288597646
H	0.87668166504619	6.11182003320848	-0.87771857612245
C	-0.49510329899498	5.16735412626295	0.48135070617040
H	-0.88557827466713	6.11084583056780	0.87518265353231
C	-1.03345418995347	3.93442165320714	0.98523643114065
C	-2.03949651646032	3.85029220917737	1.98689466373761
H	-2.45375613265234	4.76660515703516	2.42035852375340
C	-2.47637968653755	2.60750644456322	2.41612429068105
H	-3.22974954174615	2.52661954123310	3.20419961691056
C	-1.96449082543607	1.41111894431963	1.83666181683576
C	-0.53391648251313	2.70257907465006	0.47923669390538
C	0.52999624792106	2.70317262444617	-0.48061200318481
C	2.45483499154449	0.06563379427439	-2.30117815680466
H	1.88470383956515	-0.72262625815445	-1.77929633004231
H	2.21333367194786	-0.03240428563826	-3.37858085662993
C	-2.45469163506210	0.06279662997398	2.30088162155770
H	-1.88375767440335	-0.72478411126337	1.77883424257823
H	-2.21253133523553	-0.03475853656097	3.37818536541789
C	2.88487938580620	-0.10168159930579	1.73801599628847
H	2.41406374999722	0.69255565522818	1.13433397933934
C	3.97134397782169	-0.06863469949209	1.53512666069049
C	-2.88636930104252	-0.10328224015699	-1.73801303419804
H	-2.41946473884683	0.69069899545445	-1.13099668141687
H	-3.97351183420830	-0.07355127695222	-1.53836594841306
C	-3.97562061066239	-0.16680714982797	2.11883846051142
H	-4.24029753452637	-0.06412224094106	1.04870609773866
H	-4.53694424939072	0.62515102090439	2.65002705564023
C	-4.42466363725673	-1.54325728583819	2.64129685363758
H	-4.13788087180416	-1.63819262124101	3.70652787188799
H	-3.87094746236582	-2.33692838172740	2.10146256466888
C	-5.93640687676439	-1.76809007802647	2.49101398686349
H	-6.25233708033890	-1.70640826848265	1.43421841128001
H	-6.22685171042012	-2.76184398589736	2.87016089609223
H	-6.51212463861947	-1.01515614042563	3.05707001866702
C	2.65255912782662	0.18336242588546	3.24827295165851
H	1.56663423559452	0.14821609376061	3.46430456031215
H	3.11308259209709	-0.62299862836112	3.85004810407203
C	3.23140226961041	1.54284689643485	3.68010283871649
H	4.31318672419241	1.56756059766351	3.44664556615833
H	2.76676227240243	2.34708017009281	3.07564474819627
C	3.01858923902073	1.82526964043541	5.17477166888142
H	3.44085311287930	2.80513962679478	5.45305025913130
H	1.94543497386276	1.83531341678393	5.43690225201868
H	3.51024744666306	1.06124085740037	5.80183492509713
C	-2.65009192801709	0.18594522880313	-3.24687771060533
H	-1.56327259764008	0.15568602050486	-3.45912571237394
H	-3.10524135965556	-0.62098747879230	-3.85197208950549
C	-3.23298638172866	1.54396674240994	-3.67785573652731
H	-4.31579403196032	1.56346692801653	-3.44872792487767
H	-2.77430967390262	2.34879166215034	-3.06964986204700
C	-3.01538316626033	1.83080260380380	-5.17099662148108
H	-3.44079481130871	2.80946797816194	-5.44871775048939
H	-1.94123154139600	1.84614569179202	-5.42876395260491
H	-3.50116243114679	1.06610892728439	-5.80182136221166
C	3.97595099347688	-0.16201192521617	-2.11829085729507
H	4.24001447473412	-0.05810023786759	-1.04812825672307
H	4.53662558035139	0.63009326643895	-2.64993760836174
C	4.42670637825780	-1.53846771852024	-2.63928409471000
H	3.87360182196032	-2.33218611071090	-2.09887912989044
H	4.14042453326197	-1.63473233013493	-3.70452948971537
C	5.93862594163241	-1.76154106793850	-2.48818127050931
H	6.25404855752938	-1.69850694695868	-1.43131210435759
H	6.23030089653856	-2.75533924198374	-2.86626843452322
H	6.51375468983020	-1.00851776389855	-3.05471302854234

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Bis-dbp triplet

Cu	0.03706848776816	0.06274884404396	0.02766844129090
N	-1.02338674283384	-1.45508263440139	0.76120009337574
N	1.23232072352653	-1.37232737804697	-0.67193213407868
N	-1.15985678511793	1.47321693862331	-0.71523218857347
N	1.08970994858455	1.60223774707228	0.72643847568735
C	-2.06511135632618	-1.43117044454535	1.63271738284760
C	-2.59167025585706	-2.63344251153020	2.15506667161440
H	-3.43316726808225	-2.57663945999294	2.85115871124959
C	-2.06198769508095	-3.87374275575103	1.78207795581583
H	-2.49422731991003	-4.80373242145507	2.16513720418040
C	-0.94440480697183	-3.91773163645135	0.91900781417228
C	-0.29073591885648	-5.12555434616350	0.48978388046581
H	-0.68658909368711	-6.08499425238775	0.83870914190784
C	0.80072909079629	-5.08692862102519	-0.34699775532232
H	1.27391605989575	-6.01579062162842	-0.68208873790892
C	1.35420782826579	-3.83616249324160	-0.79395817668460
C	2.46583799796541	-3.71424080586511	-1.65700055141183
H	2.97244426752519	-4.61152583866911	-2.02671411514436
C	2.89542528952913	-2.44057256483628	-2.04538881204658
H	3.73230400082667	-2.32612411313300	-2.73984156018114
C	2.27320923237225	-1.27730181697421	-1.53984648656086
C	0.73807522452232	-2.62707813526080	-0.35013900709926
C	-0.42873387811270	-2.66935112758460	0.45639265430785
C	-2.21196123865330	1.35336107567146	-1.56547584978581
C	-2.85529373918158	2.50095596474463	-2.07948216047547
H	-3.70794752436202	2.36423879526617	-2.75050771038802
C	-2.42779834972298	3.78580641530346	-1.72465158273404
H	-2.94985235585154	4.67191633833840	-2.09977457306827
C	-1.30619764971819	3.93237605233288	-0.87955895485963
C	-0.76043247020701	5.19669242642177	-0.46126711540161
H	-1.24347651041778	6.11446563451198	-0.81243223892824
C	0.33564240203789	5.26125906090305	0.36694440914981
H	0.72842380127561	6.23077884636238	0.69050824674123
C	0.99963291066791	4.06754907456679	0.82020428796804
C	2.13063137054522	4.05339130048078	1.66541757360692
H	2.56531842310733	4.99585552940996	2.01363865196850
C	2.68067106432165	2.82612132598601	2.05427582828739
H	3.54336601422769	2.79124256986613	2.72551005155741
C	2.15038239964938	1.60818853077362	1.57480975148744
C	0.48755726770253	2.80467057701948	0.39296124829444
C	-0.67685982484280	2.73694803573295	-0.41620041380393
C	-2.64045290793894	-0.02632227628297	-2.00405143618995
H	-2.46097089004130	-0.75338512521567	-1.19437286279235
H	-3.72745050078838	-0.02053091427218	-2.20365768715970
C	2.71016116363541	0.28805163141382	2.04693542894631
H	2.60124222880430	-0.47254239263008	1.25557615416465
H	3.79147566167060	0.40379392361199	2.24365573149698
C	2.74258216014760	0.09606225172176	-1.96418473189383
H	2.05371939502827	0.84985278121892	-1.54575468907280
H	2.65444240188811	0.16308240005527	-3.06685424143855
C	-2.63736162035251	-0.09363445443854	2.04423004171951
H	-1.99479684651868	0.70614101641701	1.63721005050911
H	-2.57493622577199	-0.01977913247774	3.14809765535086
C	2.01390514161156	-0.21243291104056	3.33944973033956
H	0.93258943429484	-0.34425489235467	3.13736260766748
H	2.09058034553037	0.56755648462534	4.12116263646215
C	2.61018587108348	-1.53127924217817	3.85960606620745
H	3.69164185633906	-1.38994718360744	4.05122691831394
H	2.53617459615491	-2.30237148426992	3.06808927125801
C	1.92092776297671	-2.03174555441265	5.13762992508368
H	0.84468585329795	-2.21550127457027	4.96752160829429
H	2.37052202279105	-2.97604570559966	5.48890073286583
H	2.00945489267216	-1.29484088028141	5.95570725867093
C	4.19884373452955	0.43372766055838	-1.56747678596024
H	4.30414745641234	0.37408462720246	-0.46760720033120
H	4.88319198517761	-0.33059106310483	-1.98325101295470
C	4.63234954955075	1.82657924298444	-2.05606306165000

H	4.51488867555091	1.87849179498782	-3.15622500622426
H	3.94678091584483	2.58915903401363	-1.63777113189844
C	6.08047252461910	2.16727513906954	-1.67499331615033
H	6.36297688104719	3.17013091763531	-2.03778898629847
H	6.22104118319878	2.15551833418314	-0.57906746345082
H	6.79118161473182	1.44226549528289	-2.11026416979316
C	-4.10593493834306	0.14040501870660	1.61950455539299
H	-4.18388318076391	0.08190268250126	0.51736673055855
H	-4.74029881718664	-0.67537487519070	2.01650163375476
C	-4.64944902980160	1.49467096587486	2.10666242309918
H	-4.55569198681707	1.54847724676620	3.20898790078062
H	-4.01457583238722	2.30807887880964	1.70427076124721
C	-6.11180936088708	1.72992607348146	1.70103187557068
H	-6.47404555617771	2.70711982180282	2.06303230230497
H	-6.23181419640813	1.71414547817586	0.60272647769513
H	-6.77442257165111	0.95184997709600	2.12025214333515
C	-1.89669530863483	-0.48840839639617	-3.28441837049188
H	-0.80771575271218	-0.50668314645305	-3.08134695506305
H	-2.05014727493821	0.25968540409665	-4.08576701148033
C	-2.35853950372969	-1.87307657161250	-3.76905937165098
H	-2.20523347639208	-2.61295677316830	-2.95924467219267
H	-3.44926588020891	-1.84628720690745	-3.95851247846726
C	-1.62640174737346	-2.33341754810921	-5.03833187935141
H	-0.53664847398373	-2.40481981117801	-4.87026139861514
H	-1.98058781182418	-3.32615022112160	-5.36436796544682
H	-1.79065913427632	-1.62921582790693	-5.87333678359135

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Bis-dnpp reduced

Cu	4.12094726679301	4.08559285921913	4.01238134707333
N	5.09515188407125	2.63380828345862	2.99870582982365
N	4.4577783379148	4.88850849389313	5.83540949385265
N	4.60541309243489	5.20815188652549	2.40347912531195
N	2.32507077342132	3.62227312889954	4.81475661698335
C	5.25258308458898	1.32325730659927	3.30151549516918
C	5.83749530299660	0.42649200498107	2.36733101846858
C	6.33238248735217	0.88815300603795	1.15488206326001
C	6.71727607464539	2.84919848115669	-0.37839813755579
C	6.56516956029145	4.19200137263308	-0.63108491667826
C	5.68368843080931	6.43563438226411	0.09951231692134
C	4.97341558174251	7.16642802292153	1.04266508810031
C	4.40364656091965	6.52801049119630	2.17703633538718
C	5.53310461920734	5.58892966571987	6.27411538643740
C	5.53506516634977	6.15388752542207	7.57525297559090
C	4.44738133939162	5.98939762332900	8.42573522227102
C	2.13619481886149	5.04164712381062	8.77684708336105
C	1.06968944150085	4.33271892033090	8.27668283355289
C	0.03035561748203	3.07802942169516	6.35093096932773
C	0.14895251136226	2.62169362731584	5.04283819280887
C	1.30709105892565	2.90685532621216	4.27499816888717
C	5.55248393531352	3.09194009626664	1.78744822706941
C	6.21674566909457	2.26478446260903	0.83568286010550
C	5.86983357516433	5.04364619446057	0.29480985122065
C	5.33442228842411	4.48488297148413	1.49162108339810
C	4.75190509216021	0.85954544588380	4.64952219294294
C	5.81340917994390	0.43540042396928	5.72420218863859
C	6.59947980703251	-0.82460613445473	5.30388378165486
C	5.03078826958009	0.12582127220654	7.02054431426065
C	6.79816058106086	1.59357847600808	5.98123333490546
C	3.58148908410688	7.28645439499385	3.19252979711175
C	2.15519156855921	7.78052761682457	2.76353482699099
C	1.30502424996416	6.58887718367990	2.27950580241461
C	2.21824033528216	8.85206517296364	1.65443645397525
C	1.50576935299162	8.40110397511360	4.02119388117780
C	3.36543667049148	4.75445619373861	6.65308761254671
C	3.31087653028989	5.27131560714647	7.97930743072808
C	1.09005492836914	3.81437373567053	6.93520026923348
C	2.23343817316381	4.04209504212480	6.11677416390570
C	6.64960808834624	5.73642845222657	5.25660942129604
C	8.13630536417047	5.96678901597065	5.67380117721611

C	8.97960085069776	5.71712574489630	4.39866554150544
C	8.59278063350531	4.97306887956465	6.76388629335252
C	8.39637311677851	7.42447803985979	6.12429995251931
C	1.55364622709784	2.42775121212228	2.85589665476963
C	0.38904864278576	2.11419488725060	1.86466108948787
C	-0.65665513190678	3.24937766576035	1.82312610537573
C	1.04120824649285	1.99694888612254	0.46446710708354
C	-0.29122881085731	0.75892081824802	2.17437840909831
H	5.89786912591004	-0.63493000625401	2.61876327602462
H	6.80294870897951	0.20130944812576	0.44335734885806
H	7.23278691801144	2.20330946785885	-1.09677910559122
H	6.96441427365465	4.63340410884866	-1.55019637240135
H	6.10491053275989	6.92281473790879	-0.78631032358070
H	4.84020510751417	8.24370675222466	0.91910086075280
H	6.40367108046947	6.71936102342045	7.91384060525033
H	4.46127796367123	6.41549950328772	9.43454990428671
H	2.10949395331058	5.43963462234981	9.79659520538659
H	0.18216495790724	4.15570924000212	8.89309392459638
H	-0.87289119166319	2.86716566442772	6.93329155286332
H	-0.66068184847354	2.04201014288618	4.59867476557266
H	4.06075930537065	0.00628579018864	4.50139218682292
H	4.16273082498674	1.69563079469670	5.06699453239354
H	7.24739274025350	-1.15977083840494	6.13311987418041
H	7.25603749068850	-0.63521308267607	4.43710139362155
H	5.92316982467472	-1.66291740359820	5.05371379489392
H	5.72226917630142	-0.16516401452921	7.83088475284836
H	4.31900089835327	-0.70656889821995	6.87243681774205
H	4.45797126022251	1.00589979566502	7.36478635633111
H	7.37408081235247	1.84366016589613	5.07187381514076
H	7.52072818117586	1.31888137569551	6.77023066819836
H	6.26749786617255	2.50408895963224	6.31185724639775
H	4.15725795096543	8.16937089791619	3.53372397764242
H	3.46007595273002	6.61339939866413	4.05997885580581
H	1.22107102199240	5.81343334583804	3.06163145239582
H	1.74101058835382	6.12128909576696	1.37816500713346
H	0.28348803804247	6.92168823285557	2.02306649759618
H	1.20932452729305	9.25926934985800	1.46458287003368
H	2.58540357068522	8.44002783936725	0.69855508991526
H	2.86755602903586	9.69956768203597	1.94227194630172
H	1.43012097086447	7.66312563754987	4.84025148525876
H	0.48627658792627	8.75987744110982	3.79444578873342
H	2.08961734246363	9.26296108559851	4.39230458204630
H	6.36153798394952	6.56726066291026	4.57808601866548
H	6.58807000991530	4.82911238360143	4.62479390325351
H	8.67264168747409	6.38735701283390	3.57486257399289
H	8.87499577123681	4.67476016650439	4.04681139888591
H	10.04989804454402	5.90013248000165	4.59869614767102
H	9.66835909477188	5.10737313243897	6.97570697273563
H	8.44439753205337	3.92850471911129	6.43755313665725
H	8.05042159209696	5.10686776740596	7.71551480855664
H	8.07682792733757	8.14364595337240	5.34813539232114
H	9.47581950750288	7.58007797904966	6.29801080101937
H	7.88036392276822	7.69545436664641	7.06081542105012
H	2.18464541670657	1.51643726786788	2.92759764767739
H	2.21787010443263	3.18947658158990	2.40351459743303
H	-1.18187983731077	3.37937346894007	2.78483703925045
H	-1.42157796610284	3.03533481880038	1.05576914127387
H	-0.18579409179567	4.21457132857611	1.56546125895914
H	1.81915771027698	1.21173667196291	0.44636727852840
H	1.51152971598265	2.94954356030411	0.16018414042031
H	0.28423721756695	1.73623538037954	-0.29585038478678
H	0.44987374124678	-0.06071731927121	2.20135564932720
H	-1.02734370013791	0.51621027285144	1.38773078391886
H	-0.83453095251454	0.74708930179701	3.13423330739776

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Bis-dnpp oxidized

Cu	4.07614506802831	3.95437531027326	3.99139411578470
N	4.95274317997655	2.53767342393460	2.88153139580618
N	4.27431869468028	4.98058756012058	5.69279746375765

N	4.59694565521105	5.19629899616330	2.44909468798089
N	2.35605040125931	3.25137068607700	4.86607688160234
C	5.17950702399878	1.23588120054183	3.18172075804916
C	5.80115678682660	0.38578418562329	2.22348479622128
C	6.21786962578834	0.87849604958592	0.99855981730317
C	6.48074866728728	2.85960834780231	-0.52697037685494
C	6.29360018557059	4.20271281782741	-0.75179043233604
C	5.47594904557941	6.43002174891187	0.07199523504626
C	4.85206908010302	7.15385427988607	1.07159458515308
C	4.38850874714715	6.52236069237410	2.26328168887168
C	5.32165215986235	5.74512250827645	6.08961146220305
C	5.24890312107529	6.42743674230893	7.33409324285304
C	4.13603403190500	6.30633190429441	8.15264554846539
C	1.89160314846056	5.24077301108223	8.56898637163291
C	0.90457032343560	4.38422469870348	8.14228735133615
C	0.06139508821910	2.75066760454645	6.42740422884932
C	0.26487330183699	2.11024940013566	5.21858122585641
C	1.41979285520638	2.37573010387178	4.42519703957850
C	5.39829276370173	3.05397237265454	1.68754738550689
C	6.04325449397785	2.25570756667131	0.69915063014948
C	5.66247730136704	5.03263473723741	0.23496016529884
C	5.20443994286199	4.45928548083612	1.45651998689273
C	4.75153691833730	0.69132557472421	4.51891840102515
C	5.88931366950458	0.41555848510436	5.57539111920708
C	6.87435676704392	-0.67266004638001	5.10072539799616
C	5.17799634252121	-0.07104159406272	6.85843167052843
C	6.65671930275321	1.71834650014613	5.87110088823993
C	3.72041326451589	7.35689593745521	3.32888793160229
C	2.28351902867220	7.93755290290383	3.03820423736683
C	1.29833379282654	6.78434384199611	2.77585145120164
C	2.26314208359806	8.91689897278219	1.84610357426238
C	1.86619520217867	8.69930940349446	4.31735790316677
C	3.18646166423168	4.80701668257095	6.50987144112143
C	3.06073867128863	5.46502235305730	7.76659411663629
C	1.02346270834037	3.68489384641532	6.89313131533465
C	2.16364337792579	3.89980397807233	6.06715888348580
C	6.49941455783698	5.84806367980638	5.14106890588407
C	7.96339382203089	6.03996657824175	5.67472107232858
C	8.88665231133782	5.68437991343234	4.48251073808228
C	8.28254445697992	5.09094177347041	6.84901695568069
C	8.25449477041120	7.50919692856215	6.06552989389067
C	1.62326778809278	1.62213209425327	3.13427891879550
C	0.68334456076630	1.94373314144286	1.91099642704724
C	0.83015591414354	3.42414739790848	1.51535616580027
C	1.17013237574367	1.04313170558487	0.75231367244062
C	-0.79989279657071	1.62975193937826	2.19764872884225
H	5.92793509302511	-0.67069822378226	2.46926583576277
H	6.68193260962165	0.21693143749023	0.25960678100792
H	6.97188110024456	2.23132169441093	-1.27636472743337
H	6.62818867907898	4.66320003556235	-1.68649124791116
H	5.83653181121682	6.92543956651876	-0.83551642608503
H	4.71996132166264	8.23291336906425	0.97250872593991
H	6.08254167577001	7.06016721470064	7.63756215581203
H	4.08676371095381	6.84833103489143	9.10289048750913
H	1.80524237108299	5.75742138098150	9.52980735624347
H	0.01414776812816	4.21197835942324	8.75479382542081
H	-0.82257021069134	2.53025433415669	7.03489946333405
H	-0.44852420534969	1.36540991984253	4.86092741083128
H	4.21172797712450	-0.25969648424824	4.35168750632748
H	4.03960633577411	1.39889966640001	4.97596679852906
H	7.58526108118505	-0.91211732995738	5.91017694654188
H	7.47413308402385	-0.34821791674946	4.23242121095662
H	6.35209376243669	-1.61043130756810	4.83764408501217
H	5.91721370593927	-0.27013934636481	7.65324707703803
H	4.61955244307189	-1.00722042527483	6.68119383785329
H	4.46799483230964	0.68456612213163	7.24164021838443
H	7.19353232406106	2.09040758210477	4.97909399080777
H	7.40861457133245	1.54906482025537	6.66123503739281
H	5.97631019734637	2.51428591753089	6.22821516668278
H	4.38334862087063	8.21749055230875	3.54480878995287

H	3.64970681466618	6.76057807404641	4.25088687050781
H	1.28135089507764	6.06984246195121	3.62052477520499
H	1.55803524906377	6.22923269408250	1.85756904069678
H	0.27290056227572	7.17248099100959	2.64897601418675
H	1.26842758536924	9.38891794083499	1.77022185601413
H	2.45035147626842	8.41234308235267	0.88237444408947
H	3.00062125065512	9.73103932421444	1.96940461214380
H	1.85426106875688	8.03483438173062	5.20079035669222
H	0.85157145090063	9.11672297015007	4.19902833858622
H	2.54954672546814	9.54062259838319	4.53026615629380
H	6.29373823760899	6.68455000537303	4.44210420662681
H	6.47423778812803	4.93422563389742	4.51849852910392
H	8.67884334845199	6.32184429278272	3.60368499767342
H	8.76623716155387	4.62807397020055	4.17950376972331
H	9.94429209122113	5.83371122361538	4.75828144264945
H	9.34355721443547	5.18970106176010	7.13567659141488
H	8.11097722482758	4.03592972043812	6.57156594246528
H	7.68167030482056	5.30672463700487	7.74944226457297
H	8.01393110267884	8.20144753287957	5.23847393852421
H	9.32762321851902	7.62764221697505	6.29352560678744
H	7.70736362244201	7.85156402106320	6.96019338036490
H	1.51278320487676	0.54373609946722	3.36087570946549
H	2.65913697808559	1.77918293680306	2.79856876775402
H	0.46430755811712	4.09379506679169	2.31285149347424
H	0.24431780200240	3.64196012346500	0.60562825153252
H	1.88480426997751	3.68246764080403	1.30153005457360
H	1.07011849559458	-0.02838190802954	1.00125218876632
H	2.22873315504039	1.23976300534860	0.50153211481779
H	0.57089935879434	1.23111353706802	-0.15503644734697
H	-0.94128913688736	0.58836053041766	2.54021938354580
H	-1.39120174975636	1.75056320436599	1.27362943177850
H	-1.23769623713050	2.31164553482280	2.94725054643004

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Bis-dnpp triplet

Cu	4.05974210614241	3.94461195571288	3.98854807424292
N	4.90458412461756	2.52436078958436	2.88826126335661
N	4.24614273172215	4.96933414248697	5.66977139477926
N	4.60622918607916	5.17668882984021	2.46711302387996
N	2.35731210504641	3.22584664585930	4.84720636704241
C	5.15039083759520	1.21934551155997	3.19734772831284
C	5.76106741402346	0.36489828969917	2.25323822861073
C	6.16325578128822	0.84329366956883	1.00256819763684
C	6.39895541661097	2.80786769098393	-0.54557503723155
C	6.20646110123022	4.14720556484663	-0.78114512135017
C	5.42593920664315	6.38559043841772	0.04078412790609
C	4.83468721103890	7.12535919475752	1.0655056717058
C	4.40845459006400	6.51032379951085	2.26696808751471
C	5.31387335838779	5.70859606074791	6.10088836644679
C	5.25627394090472	6.34744800971761	7.35456910700533
C	4.12840204972212	6.23173698398319	8.17778462036630
C	1.86311622831667	5.20010120755284	8.55665512739367
C	0.86245968349057	4.37241556284365	8.10833957560066
C	0.01459044738412	2.76860131590181	6.37313886741460
C	0.23463656856043	2.12291747909473	5.15588281333870
C	1.40347482133600	2.36541241977823	4.39436607873013
C	5.35863592793405	3.03150890071393	1.68112660242300
C	5.98670055764618	2.20922522410594	0.69436529425847
C	5.60250867655932	4.99655536785421	0.20906514242952
C	5.17437802431476	4.42367011831901	1.44753597503103
C	4.73033294957732	0.69868402314290	4.55221709028045
C	5.86913547570660	0.45713753748292	5.60837297572806
C	6.83611317908929	-0.66357691555805	5.17333037949181
C	5.17054959792457	0.03713191753462	6.92145693208266
C	6.6607755673424	1.75903080816386	5.84139821681431
C	3.78869736982536	7.36101685797648	3.35568504586267
C	2.33831936017708	7.92393170775013	3.13189006826926
C	1.35210481444157	6.76245090254104	2.91117910179474
C	2.25598748744897	8.90080823752117	1.94030787388704
C	1.96303223137477	8.68315616173408	4.42526565435081

C	3.16001657638077	4.77532459294080	6.50260961136518
C	3.04801189617085	5.42074976213448	7.77188300938789
C	0.97786051778948	3.67887666168991	6.85424627839587
C	2.14302761434843	3.88807449570941	6.05141133452392
C	6.48365104811102	5.80961452880444	5.13745680437499
C	7.94295258275291	6.07427973846454	5.63474328377062
C	8.86097126699163	5.75197255311529	4.42878654030620
C	8.33737734001768	5.15268965910267	6.80878996756518
C	8.17404398250849	7.55949824323759	6.00494900193553
C	1.62800655490529	1.59801031190945	3.10941215717886
C	0.74816835686389	1.95022771745047	1.85635387323837
C	0.92775794817455	3.43460899555631	1.48855096962703
C	1.26529374580892	1.06388173128859	0.70000744629371
C	-0.74975369896513	1.65411780526101	2.07869800446502
H	5.89299779343707	-0.68817672896307	2.51108767998106
H	6.61571197924873	0.17159567145428	0.26601491671393
H	6.87374064130428	2.17186477137175	-1.29982790766167
H	6.52223403617506	4.59654191917433	-1.72840794471603
H	5.76447185983516	6.87299911848650	-0.87919110046401
H	4.71478127651250	8.20599821844666	0.96586558430288
H	6.10090432579620	6.95332686542090	7.68083791913668
H	4.08779542579251	6.75481025291172	9.13850349665010
H	1.77635817479006	5.70497755015659	9.52436069880835
H	-0.03792712771621	4.21170795583689	8.71033490320214
H	-0.88321750070321	2.55897258838082	6.96365705741134
H	-0.48055424698276	1.38512351741170	4.78701095835641
H	4.19141759768206	-0.25756424348158	4.41180769787502
H	4.01526871154118	1.41244952087714	4.99356647500361
H	7.56326555213419	-0.86895203461819	5.97872234956168
H	7.41334474909483	-0.38808695865272	4.27391382528095
H	6.29754315056835	-1.60670801577004	4.96634815629855
H	5.91650883624273	-0.14587275945818	7.71484250543697
H	4.58824372022123	-0.89254029125771	6.78835442101184
H	4.48121400355694	0.82250869465161	7.28117446726923
H	7.18759545450160	2.08280547252755	4.92541014156513
H	7.42071948930889	1.61256206102413	6.62937598784282
H	5.99664598329527	2.58030042204572	6.16745259943625
H	4.45556860721434	8.22867983803917	3.52698234520500
H	3.77107909694263	6.78037293350751	4.28944206806416
H	1.38235470811893	6.04515436654079	3.75204711677822
H	1.58211581836178	6.21385204609968	1.98164262156511
H	0.31720984332523	7.13969045371410	2.82946606309155
H	1.24816562162270	9.34985334339083	1.89156607159697
H	2.43418460859864	8.39633545028967	0.97513652521211
H	2.98116090009912	9.72948160921646	2.04121830038750
H	1.99033033311540	8.01727605926296	5.30679492606321
H	0.94236137881994	9.09730657008217	4.34702121031063
H	2.65282346139871	9.52584707271888	4.61350354611966
H	6.24578758428255	6.59507193681292	4.39178561735053
H	6.48271325456189	4.86645276666448	4.55785995898703
H	8.60048070594764	6.36642125382509	3.54752755304449
H	8.78385922848050	4.68866268546587	4.13735403345261
H	9.91640689363520	5.95639365412229	4.68000502009924
H	9.39924908731731	5.30536073577389	7.07103660922859
H	8.20984129359223	4.08928526862081	6.53911520426914
H	7.74129866586241	5.34168420665440	7.71742362866684
H	7.89787356546255	8.22550968714621	5.16715559915799
H	9.24224763868343	7.73032795186689	6.22684913754620
H	7.60759429821421	7.88852104701546	6.89205090010834
H	1.47673316591550	0.52339655354249	3.33083767623902
H	2.67894186608788	1.71872770961182	2.80972759827565
H	0.53504387706120	4.09274080321982	2.28242904983323
H	0.38536431117697	3.67428963983226	0.55672047056934
H	1.99334734880661	3.68417226463211	1.33020990415178
H	1.15214423065356	-0.01052156163529	0.93298914099199
H	2.33318368994354	1.25634540453829	0.49046790395939
H	0.69812023502523	1.26707704178127	-0.22541033183400
H	-0.91670207767936	0.60567478084096	2.38789341794334
H	-1.30834147950884	1.81309910758745	1.13930069238868
H	-1.19649349759350	2.31878054284580	2.83871943957357

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Bis-dsdp reduced

Cu	0.01513180865582	0.03236201334118	0.01545247126318
N	-1.50309189150907	-1.06897477440490	-0.74394519825059
N	-1.48134131615164	1.20284088119839	0.69169585878008
N	1.50222737523842	-0.74039693936011	1.14458444022523
N	1.54202158412294	0.68959150205107	-1.13042817269192
C	-1.47176428728266	-2.20711997723479	-1.47200270817101
C	-2.66906469370407	-2.81006673044196	-1.93956174111502
H	-2.60665403638020	-3.73070654685822	-2.52645466666171
C	-3.90403491043526	-2.24250065750259	-1.65787107486074
H	-4.82965492001025	-2.70537327849418	-2.01636019937531
C	-3.96265817888875	-1.04679991588050	-0.89661304990323
C	-5.18736976754938	-0.37818390886799	-0.55152967590756
H	-6.13407650562279	-0.81205697160329	-0.88996324031094
C	-5.17628996906120	0.78180359316165	0.18663812453759
H	-6.11402244500667	1.28502982793107	0.44439222506982
C	-3.93955526225323	1.36088606760760	0.63524404687101
C	-3.85791555872706	2.55546425246716	1.39630043876717
H	-4.77401866391827	3.08804170312680	1.67309493447543
C	-2.61290638522265	3.03313103931897	1.78243001466846
H	-2.53336149781901	3.95111963565256	2.37145041973063
C	-1.42833788988628	2.33926745222922	1.42185936758007
C	-2.70962318342809	0.71912959583728	0.30852633781992
C	-2.72104217602565	-0.49718443751255	-0.46333197814109
C	1.44069852734180	-1.46497823912606	2.28409384670062
C	2.62042143974208	-1.94789310288475	2.90886415362457
H	2.53368387512779	-2.53193745675701	3.82931095719339
C	3.86931346535352	-1.68244108508665	2.36416973099140
H	4.78149730681427	-2.05184361272390	2.84476677675421
C	3.95993227235973	-0.92191454192221	1.16998818342308
C	5.20156498148615	-0.58913294247073	0.52669691346987
H	6.13560092407708	-0.93744116437700	0.97978772371019
C	5.22206503088867	0.15008283561081	-0.63250814491971
H	6.17261715264150	0.39883260018684	-1.11582603269924
C	4.00208256682074	0.61095608848907	-1.23689360582004
C	3.95223108947019	1.37322100726930	-2.43246697889097
H	4.88184834177304	1.64280710340243	-2.94496996473966
C	2.72094746310276	1.76855642447382	-2.93729221852644
H	2.66572222826499	2.35756483632883	-3.85708635039418
C	1.51878865354515	1.41675827320299	-2.26934517718305
C	2.75593840088499	0.29582987930569	-0.62104095880560
C	2.73446304355824	-0.47542133459863	0.59554415273861
C	0.06512133477357	-1.76075027563272	2.85433385096004
C	-0.30564968993742	-3.25237102185479	2.62195605270526
C	0.10716441532504	2.57322546668525	3.39990080472894
C	-0.11104214613761	-2.79870126866774	-1.79480379990061
C	0.22068125226254	-2.59105130142836	-3.29946457769003
C	0.16361100026109	1.87177794116401	-2.78098271584507
C	-0.00484987064392	3.40006241279322	-2.55128587163949
C	-1.42296835931075	3.92252902384065	-2.82557744811193
H	0.72349797588250	3.94180650058179	-3.18586248822869
H	0.27235479122294	3.62604434297015	-1.50515765281870
H	0.39770613572474	-3.89118748352778	3.19106448470188
H	-0.14076563214503	-3.48820557368985	1.55459967692816
C	-1.75123099557488	-3.60468902688379	3.00328443613602
C	1.53521353211722	2.80107213651297	3.91784854770179
C	1.65219391278225	-2.99041874171768	-3.68726761497170
H	0.05935191765723	-1.52524537075126	-3.54532650500754
H	-0.50512670063042	-3.16163298213602	-3.91125418350208
C	-0.05965249288856	2.81604355759282	1.87327170983499
H	-0.59836869646374	3.22902517062042	3.94659999722529
H	-0.20322512967658	1.53621536820118	3.62403146012910
H	0.66365383001533	2.16628919771348	1.34156398631814
C	0.20557480698574	4.28858194847157	1.49737315163027
H	0.61410003845381	-2.20657587895110	-1.20278714663810
C	-0.01019504398357	-4.28328718960708	-1.38457389731580
C	-0.04159212209061	-1.37015888755666	4.34400017215939
H	-0.63627934572421	-1.14143811331419	2.26078176132560

C	-0.06803701300628	1.48538717416479	-4.25670890539879
H	-0.57779106913123	1.34720099331445	-2.14669242960651
H	0.59590012966457	2.05226065247942	-4.93384295309289
H	-1.10651551275149	1.70337282534707	-4.55473915469804
H	0.11196827243841	0.41124443170286	-4.43048261388604
H	-1.70953398272699	3.81027047417667	-3.88477894242381
H	-1.49358689924361	4.99587401167302	-2.57959934165244
H	-2.17078071644082	3.38699550693390	-2.21336950920707
H	-2.47401903609995	-2.96468058608033	2.46580032281872
H	-1.93526805905887	-3.48887738221459	4.08460527572411
H	-1.97418587364471	-4.65377361947995	2.74390705982978
H	0.32463212018683	-0.34577541390523	4.52442616517310
H	0.54411996398722	-2.05361092581909	4.98493868446663
H	-1.08907893683848	-1.41823516891066	4.68337471361119
H	1.84647801875173	-2.74858144096177	-4.74616896849485
H	1.83050112019326	-4.07147109308513	-3.56050784353629
H	2.39774055984124	-2.44959667952742	-3.07695949930819
H	-0.64306898739372	-4.92501693097516	-2.02364875663793
H	-0.32272609676339	-4.43903688242451	-0.33849182045564
H	1.02729982769223	-4.64242029184721	-1.48131904303658
H	2.26183711098627	2.16791575829282	3.37745726569053
H	1.60234683535644	2.54991607567123	4.99030953881898
H	1.85436789336814	3.85116083281273	3.80785746559074
H	0.01911550024963	4.47729932910667	0.42700674073910
H	1.25307114009292	4.55899931578206	1.70822600715925
H	-0.43585584735374	4.97647072426015	2.07711577897127

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Bis-dsdp oxidized

Cu	-0.00542294852936	-0.01003042744090	0.02978814929506
N	-1.40699722797178	-0.77159780855203	-1.18041131952109
N	-1.59062190778276	0.72899899903887	1.05073708976147
N	1.56095207225251	-0.70569386990542	1.07152444324470
N	1.41055691445446	0.86424871486084	-1.11322054947556
C	-1.25340673791080	-1.62733563843349	-2.21315986818070
C	-2.39364459481679	-2.04578112721282	-2.95682268708562
H	-2.25205547837595	-2.72793708262250	-3.79910575413979
C	-3.66236831550769	-1.59451872180815	-2.62895226347395
H	-4.53234626390650	-1.90578975378479	-3.21650079325154
C	-3.83817387214360	-0.73505403945797	-1.50983040793673
C	-5.11082246650184	-0.24472394933478	-1.05958614590457
H	-6.01116868986499	-0.53480561944027	-1.60981142143409
C	-5.20009068249321	0.57490960511221	0.04291380451303
H	-6.17133591068744	0.95616150777562	0.37275250108045
C	-4.02784131646475	0.94133167687092	0.78867040874742
C	-4.04513103273850	1.77971938475200	1.93581965418430
H	-4.99536947332651	2.18340547325169	2.30055089718394
C	-2.85740851470979	2.07964231154045	2.58320614554712
H	-2.85943449188228	2.72840555756404	3.46205067718709
C	-1.62035431849787	1.53372466410318	2.13628902847889
C	-2.75634352651935	0.45669322478280	0.37203093646387
C	-2.66197172966304	-0.36457995860426	-0.80056642646398
C	1.57437834581358	-1.55622310053401	2.12184878858086
C	2.81336971211882	-2.04553552642290	2.62451261381590
H	2.80285528554710	-2.73181937893599	3.47479407911733
C	4.01626946603787	-1.65152601931155	2.06111639113814
H	4.96634986737849	-2.01446660691468	2.46663308782942
C	4.01550182306175	-0.77473077936619	0.94217139638526
C	5.20394851740362	-0.32258722621176	0.27364113839029
H	6.17593006322746	-0.66220475586209	0.64428014922181
C	5.12761508337861	0.52525630832330	-0.80844204149579
H	6.03842767626645	0.87962231838022	-1.30072073420502
C	3.85596740608549	0.96245218025096	-1.31295828138601
C	3.69460017821635	1.84782712888610	-2.41373076836869
H	4.57636224505512	2.22054053491242	-2.94515105266839
C	2.42311982986905	2.24695246782667	-2.79262178514923
H	2.29011783057878	2.94898207828628	-3.61982826380656
C	1.26841480912093	1.74934131694388	-2.12243065448641
C	2.66483100044932	0.50874581610989	-0.68110071655348
C	2.74460095023611	-0.34404055768045	0.46945967160645

C	0.25612560662465	-2.01329610703364	2.71382834959676
C	-0.03263352728033	-3.47734039792581	2.25620332144380
C	-0.31685387892918	1.88205685647715	2.82871440996769
C	0.22274186292220	3.22638553905504	2.24517686663575
C	0.12540936462630	-2.18571520607732	-2.50849443707174
C	0.16230327350414	-3.68571085787928	-2.07538179676240
C	-0.11677855579975	2.25726652475238	-2.47460970665944
C	-0.23469709332496	3.74997706288031	-2.03123623785901
C	-1.65640698112965	4.31802709797138	-2.15316154497536
H	0.46399513451313	4.36127698935353	-2.63289981693821
H	0.10549131523171	3.83665153898610	-0.98167246426937
H	0.73905184972214	-4.14515256598366	2.68371881434629
H	0.08801981386911	-3.53327296098804	1.15714153883901
C	-1.43010503471009	-3.98400013032789	2.64361623592419
H	-0.51428971201671	4.02597588396290	2.45146466546776
H	0.27679499460268	3.13225985775081	1.14282366350531
C	1.59923298282381	3.63131572425005	2.79322604734446
C	1.56254070383461	-4.31306069067558	-2.14613066399642
H	-0.53710949285035	-4.26143318450159	-2.71052205099137
H	-0.22558408145989	-3.76501729271592	-1.04166028424522
C	-0.46270630655007	2.07018590006324	-3.96717504112300
H	-0.83297174000388	1.67322743540578	-1.86587687637298
C	0.22252760722525	-1.87183160978513	4.25079432247349
H	-0.52963464347828	-1.36724486766792	2.27503841380108
C	-0.45115403709708	1.93342070533411	4.36556364216477
H	0.40924388407279	1.09109811753967	2.56018014156866
C	0.54714062985326	-1.99987880534651	-3.98077222025554
H	0.83475499215891	-1.63486315543717	-1.86045609713526
H	-2.22506789783894	-3.32791171157484	2.24550055059259
H	-1.56108587355458	-4.05291113355884	3.73590995683463
H	-1.59308711569960	-4.99428284524893	2.23280363952765
H	0.53103791327777	-0.86593950391864	4.57991378899948
H	0.88253782972811	-2.60761980833009	4.74198922655593
H	-0.79771029209519	-2.05148762904030	4.62471094580552
H	-1.50126192411066	2.38415200654678	-4.15673244863706
H	-0.36787426746904	1.01819631526192	-4.28226512292523
H	0.18790057972001	2.68054615311666	-4.61698954284974
H	-1.99750594834520	4.36694047957676	-3.20024666005723
H	-1.68874676252020	5.34403204059347	-1.75093236318571
H	-2.38406452809709	3.71119769288452	-1.58440104931131
H	2.34828779168615	2.83394271679780	2.63609166005631
H	1.56560021280474	3.85801283667594	3.87117006373486
H	1.95964914626865	4.53887420479784	2.28091702110112
H	-0.98725317459901	1.05499021303252	4.76167264252803
H	-0.98433368398065	2.83987838674993	4.70135847554400
H	0.54605403047051	1.95900014365369	4.83278330773491
H	1.93854042380611	-4.37653410640068	-3.18042766891704
H	1.53779683184055	-5.33940121297451	-1.74424617992242
H	2.29460151404903	-3.73668988747329	-1.55192175711258
H	-0.09198901290746	-2.58370946569864	-4.66546804096696
H	1.58284755505978	-2.34571085941542	-4.12555212961446
H	0.50143814529464	-0.94339174922600	-4.29180862672466

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Bis-dsbp triplet

Cu	-0.02756100297848	0.14543930236896	0.02513857237689
N	-1.53006039726415	-0.42401994961565	-1.13749335270631
N	-1.47413106171696	0.98728997065900	1.15182603264695
N	1.37618830433979	-0.64912637385309	1.18058787018238
N	1.52817093991069	0.80625549611292	-1.07496547926578
C	-1.52006722461309	-1.28127833973020	-2.19283636390631
C	-2.72484181684854	-1.63446052962437	-2.83831374089709
H	-2.68532783845320	-2.31720993843961	-3.69076637243217
C	-3.94956120214728	-1.10806744482755	-2.41307756209067
H	-4.87707796677692	-1.35828056399506	-2.93814846217897
C	-3.98584938874420	-0.25739398272549	-1.28667049290498
C	-5.18720233469301	0.31936050759119	-0.74458293955570
H	-6.14017066976350	0.09930669524009	-1.23683694755327
C	-5.14558249314741	1.13511680388733	0.36096304741818
H	-6.06407540331810	1.58278227832548	0.75464090746045

C	-3.90611275859709	1.41236292127038	1.03712207722909
C	-3.79316803937609	2.23047422123783	2.18012421375856
H	-4.68523413909836	2.69926423668696	2.60802354825305
C	-2.53480470028972	2.43427897330331	2.75643171531906
H	-2.43495515557285	3.07301748792632	3.63626105579865
C	-1.38358214684280	1.79973686728883	2.24082501550280
C	-2.70391209509320	0.82935292381493	0.53008549563521
C	-2.74179509537853	0.03613935992532	-0.64854708447440
C	1.24343108298453	-1.52317396428923	2.21251880227405
C	2.38519173984789	-2.03393253677100	2.86777759368122
H	2.24819129496054	-2.72574286576805	3.70274666598171
C	3.67176408014124	-1.64997817917083	2.47391368842567
H	4.55288107672221	-2.02262650972158	3.00623901139164
C	3.83065323479955	-0.78523084451883	1.36896409531448
C	5.10181509019986	-0.34696349604637	0.85736734396677
H	6.01291919323262	-0.69121253050721	1.35766031503300
C	5.17732482574387	0.49018728053312	-0.23029286975415
H	6.14965240042387	0.83053020609750	-0.60144991314143
C	3.99196947459275	0.92906365384554	-0.91828303333399
C	3.99813904809181	1.77312942950946	-2.04753871718881
H	4.94734398521828	2.13751754861317	-2.45356343674180
C	2.78358588036090	2.13369320164775	-2.64187662452600
H	2.77821784252561	2.78965326444341	-3.51441637925727
C	1.55566073569549	1.63529749298039	-2.15596205286508
C	2.71947177942003	0.48862381197687	-0.43959960826548
C	2.64257934406660	-0.32807608340884	0.72081054043593
C	-0.15527655537553	-1.96530126537180	2.61077671021958
C	-0.36615396342009	-3.45199098460051	2.19867037730327
C	-0.01090700626073	2.04062522372550	2.85392886625806
H	0.57956216693828	1.12093759692470	2.69404106263342
C	0.70352696089060	3.18679221582170	2.07625082573958
C	-0.06135964848277	2.32205745472755	4.36881491611624
C	-0.19153454541967	-1.87985419298126	-2.62624863205897
C	-0.14178937080244	-3.38122277618367	-2.21622058153883
C	0.23143635729789	2.03402235012475	-2.79424822489693
H	-0.43998652521593	1.16039335262775	-2.71424424898139
C	-0.41476319601056	3.18233790398801	-1.96296010078246
C	0.35936539752408	2.40388689726089	-4.28453484144418
C	-1.80457543943840	3.61327466706612	-2.45343054958254
H	0.27185828657839	4.05081974972434	-1.96096300037832
H	-0.48966589063111	2.84059049438307	-0.91337169159752
C	0.32210529789581	-4.08961686984176	2.78620595702385
H	-0.06258673372259	-3.56886598764247	1.14071432287230
C	-1.81007756101845	-3.94742317682685	2.36952918731721
H	0.09472697985749	4.10752008649075	2.16244407541456
H	0.71336259059727	2.92010191299318	1.00274259298540
C	2.14088183506081	3.46265956188234	2.54141806625038
C	1.23116569889135	-4.03837632832779	-2.42319200880989
H	-0.91370618140282	-3.93526773390360	-2.78424128272116
H	-0.42920989748800	-3.46295850938819	-1.15048320809851
C	0.08238421560703	-1.67977909370895	-4.13202928886778
H	0.59448885735683	-1.35303709345654	-2.05351487738946
C	-0.43941476647144	-1.73093141413012	4.10930185721444
H	-0.86113820621244	-1.35308261867246	2.01881124121488
H	-1.76754565978786	4.06601596618107	-3.45835064905602
H	-2.23531166467537	4.36563803745795	-1.77090355146992
H	-2.50128369405859	2.75656739671599	-2.49103971499752
H	0.93041964130243	1.64497764443147	-4.84637372897797
H	0.85640050994229	3.38019550310184	-4.42700061933566
H	-0.63899182777271	2.47934306626966	-4.74436251628004
H	-2.52043370128299	-3.31684182188594	1.80481214045750
H	-2.12580002345707	-3.95013826671963	3.42625607041650
H	-1.90874364866528	-4.98055479115951	1.99520153508675
H	-0.22575056361327	-0.68978884108912	4.40273376995503
H	0.17289340897894	-2.39320268782479	4.74671595186532
H	-1.49777417290758	-1.93545801865383	4.33921192736144
H	2.61432778847340	4.22009939858216	1.89367339409264
H	2.76070232863770	2.54901548585327	2.49749864909184
H	2.17580587459837	3.84715478425533	3.57446714488706
H	-0.45698532907719	3.32965483199563	4.58934413348227

H	0.95203045332074	2.27172500612594	4.79825203495756
H	-0.68851902742761	1.58667291616911	4.90126670514331
H	1.51533447846432	-4.07989575483038	-3.48802299611375
H	1.22184246749889	-5.07510276807004	-2.04583432991223
H	2.02392379820249	-3.49136802396209	-1.88150224250275
H	1.10723707014998	-1.99794552569342	-4.38329089937335
H	-0.02329892571300	-0.62235337583245	-4.42632953717270
H	-0.61050716081855	-2.27362138639604	-4.75414636806665

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Heteroleptic dmp-dtbp reduced

Cu	0.01995527720659	-0.14368029208037	0.08756945665626
N	-1.70238007308295	0.66758322833751	0.89236719644938
N	-1.27405744016970	-1.32301828711611	-1.00364989650087
N	1.16831359533515	1.18834607480043	-1.04502099243716
N	1.80916922788250	-0.55937163762838	0.92857019859319
C	-1.92226166889531	1.62146257152257	1.84173561593579
C	-3.22008913544674	2.15499856793821	2.04947123428843
H	-3.36840518696079	2.92815681490379	2.80290099703090
C	-4.30275734365489	1.70235697406059	1.31717463057063
H	-5.30485766100991	2.11302569880356	1.48058525443276
C	-4.11002491926387	0.68850858206118	0.35381629745264
C	-5.20457175029596	0.17386674916099	-0.41759904328548
H	-6.20485909694885	0.58260139460876	-0.24147719987358
C	-4.99427123306148	-0.80591807409502	-1.34901700269151
H	-5.82044032518847	-1.20842128657011	-1.94406591822123
C	-3.67658405734361	-1.33009393723000	-1.56576602704878
C	-3.43526250977616	-2.33755297882392	-2.52478251316468
H	-4.26556351103817	-2.72870019723963	-3.12241748931453
C	-2.15046646529250	-2.82330273582880	-2.68770782018611
H	-1.96370916600062	-3.60973914313986	-3.41852091230746
C	-1.07438095506833	-2.32026199492277	-1.91242526457663
C	-2.55435573402816	-0.84369165134032	-0.82161177483115
C	-2.77803180792568	0.19723660319794	0.16892347328943
C	0.80950432613917	2.04390120020458	-2.02176090221783
C	1.76754264771822	2.86665345233412	-2.66927820461294
H	1.43776280940590	3.54884643210612	-3.45801909922658
C	3.10507949199854	2.80261224389065	-2.30252822881920
H	3.85266685027511	3.43303093311154	-2.79561054109213
C	3.50569320064494	1.90924511569429	-1.27660693472449
C	4.86449530098035	1.77445977993267	-0.83070760913064
H	5.63580889012902	2.39098424219501	-1.30391499509209
C	5.19188512501694	0.89074474451067	0.16894639613132
H	6.22880998477955	0.79099554459246	0.50614827624649
C	4.18656291701771	0.07718143242646	0.79600155172179
C	4.47442285493628	-0.84893032835987	1.83171144283140
H	5.50400620512419	-0.96599996553976	2.18578911241984
C	3.44235424046333	-1.59399743745676	2.38112350680240
H	3.63833620159227	-2.31446355714366	3.18095166826548
C	2.11198694122764	-1.43446474605360	1.91451043561503
C	2.82807991602659	0.18589671450254	0.37687847052489
C	2.48383307923939	1.11563436161695	-0.67419602308441
C	-0.64813716965822	2.09157730999075	-2.39858923956958
C	0.99894160153708	-2.25156051132274	2.52117015108649
C	0.32594613573512	-2.95038023067835	-2.07447215136048
C	-0.76141074709310	2.09937362682911	2.74072341253421
C	0.37413136948707	-4.02769999934783	-3.18108191844239
H	0.11617808804803	-3.62146165443511	-4.17509787516563
H	1.40390707913684	-4.41845368674830	-3.24631436761691
H	-0.28508775640564	-4.88710812267399	-2.96663041158133
C	0.70369200010691	-3.61885996714840	-0.73060899858632
H	0.69726767963901	-2.87124054758211	0.07376011232350
H	-0.00555878323566	-4.42346797680810	-0.46862445316508
H	1.71551536757133	-4.05622342998998	-0.79532161298337
C	1.35635365747755	-1.85542657176957	-2.42090401059321
H	2.37220792673936	-2.28477810776250	-2.46371669002200
H	1.13654511663864	-1.38783616805117	-3.39696401488472
H	1.33413747177587	-1.07648248339064	-1.64820813016991
C	0.39136258619607	2.63658667324173	1.86716098797951
H	0.08254508817180	3.52921211178985	1.29478886604243

H	1.25421354839446	2.91162624699317	2.49798043975293
H	0.70436864287515	1.85934185476139	1.15844114315896
C	-0.27044015296752	0.88548606790269	3.56611944988976
H	0.58292490494166	1.17913666638994	4.20238202645712
H	-1.07000870522788	0.49286724143325	4.21852631630959
H	0.05673530966120	0.08248383077033	2.89215089604139
C	-1.18404326699009	3.21408006164096	3.72366802001650
H	-1.54564596714616	4.11859535073301	3.20336948009864
H	-1.95860180587291	2.88101764838955	4.43659782446770
H	-0.30326917197551	3.51047627501227	4.31844475710336
H	0.03638068697244	-2.00475844689227	2.04473319708415
H	0.91510578979907	-2.06210206801414	3.60604225926529
H	1.18795413372924	-3.33254243293851	2.39615840023042
H	-0.83354586144064	2.82192348852968	-3.20124987679467
H	-1.26694370514566	2.36779387987180	-1.52700487127637
H	-0.99377013416213	1.10115286532951	-2.74301994044854

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Heteroleptic dmp-dtbp oxidized

Cu	-0.00242270825516	-0.05047710272520	-0.00968794456194
N	-1.68580153980266	0.71491418391514	0.87712007723401
N	-1.25562513210281	-1.39261930353365	-0.91057852344118
N	1.27578153319759	1.35952929743213	-0.71914484589811
N	1.69608209913974	-0.87670440836250	0.73946323958104
C	-1.87767987298208	1.69628297262455	1.80554693147479
C	-3.20173436411599	2.03742827759227	2.19943112528405
H	-3.34568174260794	2.84911112948158	2.91179497811438
C	-4.29996873089858	1.35863294665023	1.71256031206730
H	-5.31283549626718	1.63751766263084	2.02133222436698
C	-4.10905836907517	0.26997152013208	0.83030535700213
C	-5.21019901241440	-0.52461701777902	0.37307713621530
H	-6.21771924813923	-0.27054726267390	0.71612352383638
C	-4.99422457597700	-1.58520414725664	-0.46640055978979
H	-5.82434133179823	-2.20154086968162	-0.82466170047691
C	-3.66675591681907	-1.90104164825971	-0.90336004466826
C	-3.41583382719105	-2.97844826592050	-1.78446878137517
H	-4.24193052585834	-3.62015426420470	-2.10817716071378
C	-2.13442215293658	-3.18849529657482	-2.25118361928231
H	-1.94809873800851	-3.99237371283530	-2.96259891437823
C	-1.04538461606499	-2.37135418617107	-1.83807851517970
C	-2.54283055910509	-1.12759236073692	-0.47674029974257
C	-2.76900582397559	-0.01726709167576	0.42376744844663
C	1.02449948866852	2.38088482638287	-1.56204635711405
C	2.08960596623099	3.19586254724816	-2.03932831288465
H	1.85427882676344	4.02222056094613	-2.71613669493079
C	3.39539005498705	2.95576835436273	-1.64233201971620
H	4.21031446266337	3.59895441006584	-1.99038806600086
C	3.67986837437789	1.85372622008833	-0.78957612877006
C	5.00071371195405	1.49633626181335	-0.35318074684448
H	5.84557382197494	2.11185869684477	-0.67728565710794
C	5.20490705786665	0.40407640500627	0.46022915899132
H	6.21181180750369	0.15138497623948	0.80664038666105
C	4.10691158376493	-0.42740812501743	0.86752065154421
C	4.24004725837221	-1.55943206846597	1.71808187705295
H	5.22934832881530	-1.84912538985364	2.08726357544517
C	3.11278215972644	-2.27657227807829	2.08549207427697
H	3.19112882251201	-3.13421105558277	2.75976114164539
C	1.82988802728794	-1.92151046269657	1.58048475544023
C	2.79234879054605	-0.11072058374548	0.42324879511871
C	2.57222916091255	1.06229721411101	-0.37413608704423
C	-0.38860662282087	2.63514745240277	-2.01210987760957
C	0.60815620865790	-2.69267001103345	2.00054182282874
C	0.33337890240426	-2.64793555404809	-2.47892914283528
C	-0.71679271700523	2.47191165508035	2.46800510637285
C	0.18308252278102	-3.33995029370146	-3.86176596846967
H	-0.50634765068172	-2.79635631504252	-4.53030015494982
H	1.17231622038084	-3.35942675200658	-4.34913504719369
H	-0.14607801422514	-4.38981697031996	-3.78722844655887
C	1.14374250924687	-3.60148433163350	-1.56067373659798
H	1.37326614506845	-3.14011815369897	-0.58923062132355

H	0.59604648807923	-4.54225206659696	-1.37996975306746
H	2.09876168575420	-3.85769669518760	-2.05094517794568
C	1.10168874191868	-1.33446700949962	-2.72396543929870
H	2.10169135315059	-1.55464207201960	-3.13271603077854
H	0.57164936030357	-0.68893649895286	-3.44593063637692
H	1.24068897978253	-0.77134443062661	-1.79248695219804
C	0.48515481085562	1.54414459539025	2.73317677508594
H	0.84276245058546	1.07596748889068	1.80750556415388
H	1.32075044851726	2.12441790927748	3.15824723202292
H	0.22414926614140	0.74557898418744	3.44944368868508
C	-1.14085354949731	3.05527122508433	3.84391763382853
H	-0.24089984355101	3.44726393462188	4.34679461134727
H	-1.84148114540723	3.90251456834844	3.75770257307966
H	-1.58454234444421	2.29092450029450	4.50474847329682
C	-0.30985438022657	3.66097156248133	1.55733308130142
H	0.09025669100294	3.31995292067084	0.59154850720460
H	-1.16810332758725	4.32710912062944	1.36397515950815
H	0.47178636697765	4.25683124201549	2.05936718234037
H	-0.28825209255984	-2.36633453463699	1.45312283392476
H	0.42636809058646	-2.54752855972752	3.08134651851783
H	0.74509001777146	-3.77612642288320	1.84375635280685
H	-0.47249985961683	2.46191442581753	-3.10064108011595
H	-0.6846033393594	3.68274684626130	-1.83255573896831
H	-1.10352943127698	1.97347667842512	-1.50108310189543

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Heteroleptic dmp-dtbp triplet

Cu	-0.03482630476159	0.00340408647210	0.00262580962853
N	1.44050272454693	-1.11359349565286	0.83637013340929
N	1.44026859787353	1.11594748787133	-0.83487553985576
N	-1.51412804576741	-1.12125560269973	-0.73173923342892
N	-1.51731555775547	1.11968261340647	0.73231263613332
C	1.43837550552453	-2.13241439859222	1.75723838165557
C	2.65946323212499	-2.72374781934847	2.15270022870353
H	2.64110885038643	-3.56154612164371	2.84832395849480
C	3.88374316579446	-2.25768118849702	1.68573031945544
H	4.81984214150509	-2.73446132729118	1.99387338982268
C	3.91405175719094	-1.13492991271092	0.83907364539948
C	5.15043683956252	-0.55418295051689	0.40072476993236
H	6.08746292982169	-1.00764874320608	0.73955426960746
C	5.15036554863844	0.54245558417734	-0.41742419226204
H	6.08734109518537	0.99244778240185	-0.76099936598127
C	3.91400075847795	1.12766175052480	-0.85001287704235
C	3.88401358472263	2.24947522357658	-1.69786567916309
H	4.82045305900357	2.72221306983277	-2.01113732515919
C	2.65923529462820	2.71959415950021	-2.15952056733405
H	2.64073656131298	3.55646975440149	-2.85621061804600
C	1.43779523262299	2.13398497818000	-1.75700407533050
C	2.65941864471204	0.57503183025278	-0.43085155806913
C	2.65950663670109	-0.57709804184171	0.42665177307457
C	-1.44569716997100	-2.12014733058170	-1.65140573848047
C	-2.62238707884998	-2.68041658632103	-2.18615633993345
H	-2.53345782970637	-3.49557496604484	-2.90915624493460
C	-3.88612482351912	-2.21841523964764	-1.78545072602668
H	-4.79710156977872	-2.68209195006438	-2.17701890932815
C	-3.97521926101726	-1.13228775349569	-0.89003039792371
C	-5.20672569811818	-0.53640375296495	-0.43868538328929
H	-6.15147538386700	-0.96084390956174	-0.79408173545458
C	-5.20851710598557	0.53423393740412	0.42480042032046
H	-6.15470998041192	0.95869449055025	0.77630375365962
C	-3.97882939616028	1.13009995829413	0.88118984079473
C	-3.89366635206253	2.21642728826792	1.77679733381478
H	-4.80653221166793	2.67991756817329	2.16414794955116
C	-2.63165243380825	2.67867809627525	2.18263055468823
H	-2.54530389794025	3.49370489591023	2.90607552338941
C	-1.45288980978803	2.11863206779335	1.65235084486693
C	-2.74941827776368	0.57636473876811	0.40931810693125
C	-2.74749879306275	-0.57884991064663	-0.41298768918588
C	-0.07797274843288	-2.58893540778776	-2.07713171092891
C	-0.08686353577909	2.58668217670383	2.08451927593379

C	0.13502642729892	2.67104404023439	-2.40246369735169
C	0.13682649696675	-2.66457360226847	2.40910003454001
C	0.43042393854089	3.41974087871919	-3.73008275496699
H	1.03084413788818	2.81156261665215	-4.42854756971907
H	-0.53049787929405	3.64490898801777	-4.22327530027948
H	0.93872865273852	4.38678649720869	-3.57489934901147
C	-0.56511189314563	3.67802172137158	-1.45437131137110
H	-0.93617215930067	3.19289841706236	-0.54160047356535
H	0.11912400123432	4.49654732319305	-1.16976993856021
H	-1.43209082408167	4.12755839994908	-1.97019449437066
C	-0.81728944096742	1.50985636426628	-2.75573837270180
H	-1.75615059719616	1.90734637521248	-3.17706788242255
H	-0.36490173259196	0.83531659128383	-3.50429307545102
H	-1.07425656763391	0.91795365175395	-1.86896455536008
C	-0.81301097193326	-1.50099706231527	2.76053683943397
H	-1.07563112570983	-0.91553147404745	1.87117154999161
H	-1.74918010510079	-1.89557801955904	3.19048895791949
H	-0.35598968699011	-0.82151578684245	3.50178121586601
C	0.43612969926831	-3.40817757802501	3.73883667766842
H	-0.52313461034345	-3.62851977763154	4.23739752452707
H	0.94100450915472	-4.37734232553209	3.58578041773527
H	1.04162424928781	-2.79864500351589	4.43170593189675
C	-0.56799056212906	-3.67425634916533	1.46728308014101
H	-0.94338937921820	-3.19178808051809	0.55476524936984
H	0.11453409250429	-4.49394773809051	1.18188471318760
H	-1.43250428836916	-4.12212001180859	1.98871204068710
H	-0.15214660566683	-3.39555913762039	-2.82222840658070
H	0.51008879723556	-2.96184092175538	-1.22129144592036
H	0.49468378293423	-1.75718284564854	-2.52735014970333
H	0.47892392059128	1.75684534780896	2.54699634842766
H	-0.16405916786034	3.40007021925451	2.82190891751887
H	0.50999341352764	2.94929839673471	1.23039651531579

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Bis-dtbp reduced

Cu	-0.00010048284051	0.00013010377989	-0.02298902453145
N	-1.78146773638141	0.69184433578946	0.86823404151393
N	-1.28452026299432	-1.38820903849949	-0.98405669665665
N	1.28468873001418	1.38819660902291	-0.98412740788310
N	1.78094710988677	-0.69151110344767	0.86884792654192
C	-2.04500317241176	1.67387354502317	1.77045995025127
C	-3.38387533884217	2.06170956314914	2.05619503530943
H	-3.56654844175244	2.86544636566389	2.77116592584850
C	-4.45160665243191	1.41945418878372	1.46740253434130
H	-5.48282674853849	1.71003121295862	1.69481068368537
C	-4.20709315748344	0.34693416080046	0.57913606084825
C	-5.29638025139486	-0.38799112314860	0.00802798233539
H	-6.31826529642435	-0.09100779341225	0.26536987823831
C	-5.05253835082902	-1.44523877588694	-0.82419658387280
H	-5.87158955363171	-2.02761457440967	-1.25867214595473
C	-3.70622654223862	-1.80576120315464	-1.15591337117758
C	-3.44400222999772	-2.88382956992769	-2.02958394091746
H	-4.27798255312903	-3.46649217668932	-2.43538108474834
C	-2.13884324654518	-3.17444508984083	-2.37392975618354
H	-1.93480576737187	-3.99649266600695	-3.05976951354649
C	-1.06133175048021	-2.40375934630958	-1.86264203861784
C	-2.58361181754292	-1.08336571329057	-0.63227518892016
C	-2.84345245047989	0.01693588373746	0.29015398415540
C	1.06188381619443	2.40352857375735	-1.86309887462051
C	2.13967165189193	3.17365357164199	-2.37462552210743
H	1.93593736642174	3.99544954313912	-3.06087132399381
C	3.44470154336977	2.88282878222242	-2.03000143695104
H	4.27888915434162	3.46508210366469	-2.43595948560077
C	3.70653294564539	1.80504860357056	-1.15586959456195
C	5.05271724024258	1.44430569505559	-0.82388914237019
H	5.87196132488727	2.02633589791306	-1.25846409917999
C	5.29620826680308	0.38724439659343	0.00866301363813
H	6.31799365435061	0.09006465502915	0.26617432200173
C	4.20668555497203	-0.34725562496077	0.57985881561209
C	4.45087656481479	-1.41965658318307	1.46834625856875

H	5.48200925936335	-1.71045346447649	1.69587012414791
C	3.38295396576805	-2.06156631056636	2.05715109694880
H	3.56538417877029	-2.86525262045981	2.77224488574661
C	2.04419365494813	-1.67346003921609	1.77127983448983
C	2.84314687185087	-0.01699661938108	0.29067928570286
C	2.58366825223127	1.08311053413756	-0.63211232204637
C	-0.37253291485497	2.77470358778105	-2.30650152294890
C	0.95726279507507	-2.34792581469579	2.64470046270232
C	0.37333038030559	-2.77455274054866	-2.30563403859405
C	-0.95817900653308	2.34862665165515	2.64376856219618
C	0.38791202352591	-3.66906146457530	-3.57041882473593
H	-0.16758870461253	-3.21350034126335	-4.40902258065455
H	1.43440953866134	-3.79647754973457	-3.89693599112080
H	-0.01364123623748	-4.68102974590188	-3.38818948128151
C	1.04592158125150	-3.57073682961119	-1.15806055172160
H	1.10844729261066	-2.97207716063233	-0.23810551125114
H	0.48416431941417	-4.49563605605037	-0.93606373474526
H	2.07144055640802	-3.85738792980194	-1.45165395367333
C	1.18354364885656	-1.50623206867159	-2.62883556940782
H	2.24675030372842	-1.75826258216724	-2.78291638982685
H	0.80706524194776	-1.01546308342889	-3.54330386070643
H	1.10719012560876	-0.78601582850438	-1.80408250400170
C	0.48174513953223	2.11644163969572	2.16814074730752
H	0.70172156667556	2.67172632802438	1.24249912468703
H	1.18211324564527	2.47071890039681	2.94414880842085
H	0.68544244294204	1.05245662118484	1.98484549335160
C	-1.11911862366125	1.74251675056183	4.07000027196208
H	-0.38441539890267	2.20238024786204	4.75466201407807
H	-2.12620433913396	1.92537402980250	4.48177717445299
H	-0.95072982576573	0.65194841836219	4.06491647822547
C	-1.17741307355280	3.88472052045050	2.73171988047634
H	-1.17629213930674	4.35453644177341	1.73326302214050
H	-2.11285024767427	4.16694358637044	3.24239761326032
H	-0.35051839945773	4.32830271748030	3.31295457996140
C	1.17621604624546	-3.88405945038747	2.73268603805719
H	0.34926584625186	-4.32748937437453	3.31395516093931
H	1.17497151677134	-4.35387482503304	1.73422550950666
H	2.11162687303194	-4.16644586406569	3.24332996760784
C	1.11847700822373	-1.74178966972665	4.07088048093080
H	0.95026378886238	-0.65119858766700	4.06575364735994
H	0.38377373085786	-2.20149406046145	4.75565044427649
H	2.12558638692188	-1.92478783174528	4.48256059829521
C	-0.48268942334265	-2.11554862543350	2.16926684684527
H	-1.18298633600171	-2.46966834860510	2.94541501774793
H	-0.68627364697378	-1.05156686209254	1.98591746687487
H	-0.70288366714787	-2.67090373398387	1.24372902883916
C	-1.18348328857955	1.50660256185629	-2.62870808030794
H	-1.10773166159799	0.78707959482644	-1.80330642061870
H	-2.24650638386790	1.75917123305740	-2.78318351971316
H	-0.80717777531628	1.01479141942622	-3.54269093843802
C	-1.04468946528842	3.57235388293896	-1.15970553689910
H	-0.48245111084400	4.49718661762680	-0.93864892835512
H	-2.07007863872122	3.85922256227582	-1.45353478211937
H	-1.10745804481964	2.97463925855397	-0.23917477604456
C	-0.38640141662621	3.66813814994667	-3.57203928091192
H	0.01587457479894	4.67997360155086	-3.39064190947424
H	0.16883269718546	3.21146680885962	-4.41021683374268
H	-1.43278320554557	3.79602540767762	-3.89874000469224

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Bis-dtbp oxidized

Cu	-0.00002229084505	0.00000034525041	0.12591327447160
N	-1.73689667290478	0.79135427651419	0.83726078287904
N	-1.29557695986330	-1.37202820983484	-0.92242666105663
N	1.29527440451623	1.37213043662489	-0.92230425811304
N	1.73699471124496	-0.79184912761297	0.83645660670504
C	-1.94626639047374	1.77343321907786	1.75710886949484
C	-3.27659591367037	2.18255793968781	2.06043661466941
H	-3.42940253452905	2.98345453702129	2.78491268474869
C	-4.36516108794217	1.58507845705027	1.46490899206323

H	-5.38322201034634	1.91611744856862	1.69503785086680
C	-4.16494720937332	0.50385009620869	0.57259107804744
C	-5.27582339677704	-0.20292987189776	0.01061023908209
H	-6.28858848078119	0.12239941445565	0.26711261513441
C	-5.06251434307288	-1.27345559004965	-0.81677646440973
H	-5.89948963598481	-1.82520905115871	-1.25567851043781
C	-3.72843599849515	-1.68805563555873	-1.13111663640617
C	-3.49033930286613	-2.78029694563116	-1.99682714469376
H	-4.33582965524838	-3.34503954137409	-2.40343502032609
C	-2.19405234100714	-3.10494550718427	-2.33805842052643
H	-2.00974437025568	-3.92808399339678	-3.02739832967106
C	-1.08677339541824	-2.38297600072586	-1.81056044399450
C	-2.58754279545458	-1.00231428379061	-0.60196201831676
C	-2.81705974950451	0.12599466617421	0.27995325172146
C	1.08633442083785	2.38347267750153	-1.81000754614297
C	2.19353961419125	3.10536074668439	-2.33774351195468
H	2.00908569254985	3.92875791628173	-3.02675813939693
C	3.48990301315961	2.78033817334158	-1.99720321603132
H	4.33532792534846	3.34503934693090	-2.40400271925707
C	3.72814489477890	1.68775353774158	-1.13197886655588
C	5.06227762839979	1.27277126534863	-0.81836919761740
H	5.89916779027452	1.82449669214612	-1.25746859328828
C	5.27574339110487	0.20195391636542	0.00859461829574
H	6.28855804390278	-0.12365541747484	0.2645449555272
C	4.16497723339598	-0.50477091589584	0.57085191464395
C	4.36534401986112	-1.58627079544093	1.46281112190390
H	5.38343279323936	-1.91757492143084	1.69243442871987
C	3.27690387912744	-2.18367187203068	2.05864352767242
H	3.42983888124265	-2.98477957557029	2.78286207428444
C	1.94653223612819	-1.77420990540153	1.75594955855389
C	2.81704411697697	-0.12657132328865	0.27887497580004
C	2.58734189332117	1.00205729631468	-0.60256586040224
C	-0.32871288200946	2.79963999582868	-2.26929949335070
C	0.84000073640599	-2.41540786857252	2.62127971659965
C	0.32832670987613	-2.79856780796887	-2.27029650514217
C	-0.83953674919537	2.41468670856188	2.62216410992696
C	0.29700148835173	-3.67699043774379	-3.54765710589515
H	-0.25596165617939	-3.19791767738956	-4.37399707040359
H	1.33482434752590	-3.82711977334104	-3.89032144595699
H	-0.12347620903328	-4.68147446725121	-3.37056141428197
C	0.99318216333565	-3.63508330447625	-1.14775180758654
H	1.08483843087613	-3.06549020848394	-0.21271283429738
H	0.41213897359622	-4.55094219245939	-0.94185573100620
H	2.00505070721256	-3.94229606170015	-1.46401834187270
C	1.16302134930871	-1.54621498073056	-2.60774732050953
H	2.21406651390139	-1.82665965033203	-2.78959178416040
H	0.77880650730396	-1.04863584113366	-3.51472102828224
H	1.13598402291131	-0.81593780341251	-1.79070139004901
C	0.59069945220006	2.11122904474158	2.16258156862917
H	0.82942446103398	2.59778799718891	1.20447885634851
H	1.30197761511300	2.49272205969101	2.91412899754047
H	0.77399714119104	1.02607007023147	2.07741748745854
C	-1.03918477849286	1.83215812157426	4.05676339162986
H	-0.28072033919544	2.26567700774419	4.73155085806352
H	-2.03186272652676	2.07743986922127	4.46793262443011
H	-0.92823969198453	0.73418017891159	4.07195927053211
C	-0.99459211876032	3.96041879906266	2.69216367110157
H	-0.94961192182642	4.42616430957526	1.69375147557237
H	-1.92915441489904	4.28089264236331	3.17952640428429
H	-0.16645913621088	4.37176604030342	3.29353501220094
C	0.99470528354004	-3.96119005030478	2.69086137905548
H	0.16672062509445	-4.37246615085932	3.29248540119661
H	0.94921732815097	-4.42672353829494	1.69237816342707
H	1.92939164803780	-4.28198290527345	3.17778012555536
C	1.04035409548925	-1.83330084180389	4.05595505559726
H	0.92977283745769	-0.73528933384689	4.07148719377325
H	0.28199082466667	-2.26674926428096	4.73090096982406
H	2.03309539448373	-2.07901464147039	4.46671438769377
C	-0.59032468594639	-2.11142406088313	2.16230370431597
H	-1.30143688312007	-2.49288037315485	2.91402673819396

H	-0.77330734508658	-1.02617817512001	2.07747501514569
H	-0.82954725184399	-2.59769525981711	1.20417748239806
C	-1.16419034735660	1.54768788043632	-2.60623795677512
H	-1.13727106703362	0.81756252131698	-1.78908869041693
H	-2.21514952605217	1.82866721494159	-2.78777032703776
H	-0.78055716145248	1.04973757190003	-3.51324904000076
C	-0.99269613574896	3.63690262255357	-1.14678728188014
H	-0.41097587530480	4.55242355065587	-0.94128852355615
H	-2.00443603570231	3.94473484777035	-1.46286690164942
H	-1.08448430858211	3.06764007848637	-0.21158535404921
C	-0.29721499888250	3.67773055004927	-3.54687000192711
H	0.12385796969858	4.68203043343019	-3.37012030782265
H	0.25530649845893	3.19815236711315	-4.37321336191592
H	-1.33503792758364	3.82833426591056	-3.88932351738113

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Bis-dtbp triplet

Cu	-0.00002122856849	0.00011276258363	0.08641392810951
N	-1.73044289978426	0.73886578397876	0.82093413833067
N	-1.22342066203413	-1.41294540290334	-0.92202589965931
N	1.22357063240775	1.41297886315556	-0.92202386070232
N	1.73024403110217	-0.73844692357329	0.82152509706506
C	-1.98161356018824	1.72382747766943	1.74152966441514
C	-3.31143979268969	2.09812388328298	2.03225450188787
H	-3.48977971305687	2.89223544323358	2.75854480632964
C	-4.39442862692281	1.45707077719255	1.43865869897527
H	-5.42123645666130	1.75987208608230	1.66730633956433
C	-4.16128121092789	0.37589997066060	0.56875639916733
C	-5.24523852924620	-0.38366192430851	0.01664135372628
H	-6.26885186864883	-0.08840040395209	0.26897618833950
C	-4.99792744220350	-1.46036840824539	-0.79044001474689
H	-5.81743067858803	-2.04954099980557	-1.21480813655374
C	-3.65192866043094	-1.83572741213336	-1.11166987749595
C	-3.37918607830919	-2.91907159050541	-1.96392846016458
H	-4.20415731409179	-3.51948785023943	-2.36121243769230
C	-2.06223892708228	-3.19555391844224	-2.31672470339706
H	-1.85417418553930	-4.01226727297585	-3.00643349818788
C	-0.98953959194838	-2.42740367184110	-1.81052946459099
C	-2.53822415439443	-1.09125683322472	-0.58928286485521
C	-2.80106372519511	0.02827484036725	0.27053747675152
C	0.98985257153225	2.42716044233896	-1.81087808251772
C	2.06263559387262	3.19519991170618	-2.31706088807274
H	1.85470545755305	4.01168274722608	-3.00707866534526
C	3.37951142005395	2.91887417217688	-1.96386573852704
H	4.20455487665860	3.51919537511428	-2.36114377781706
C	3.65209574066401	1.83578088114496	-1.11123344427425
C	4.99803259779556	1.46054030935450	-0.78961385389003
H	5.81761245836073	2.04962378612674	-1.21395761543720
C	5.24519407996596	0.38404105423976	0.01778878689417
H	6.26875960302352	0.08886596790820	0.27041912186867
C	4.16113796312609	-0.37542759400721	0.56983677297916
C	4.39413226658728	-1.45639248931794	1.44002799044115
H	5.42090030920950	-1.75909875877131	1.66897913986485
C	3.31103681188323	-2.09735838800869	2.03351625198870
H	3.48924628314903	-2.89130044508451	2.76002593310318
C	1.98125723828098	-1.72319468201626	1.74240835783287
C	2.80097246559970	-0.02791912186221	0.27123590857041
C	2.53830103146322	1.09141954505927	-0.58888973990270
C	-0.43960288346577	2.77758595927115	-2.28490616512021
C	0.88825683329507	-2.38884448261722	2.61476664426182
C	0.43998991874767	-2.77814544422167	-2.28409671141502
C	-0.88870401577490	2.38958110244854	2.61391988057894
C	0.43538531368129	-3.66834756103322	-3.55292502000829
H	-0.15022684872931	-3.22072463168772	-4.37451354208571
H	1.47546034646182	-3.77606341581737	-3.90591963767466
H	0.05776522325164	-4.68765680086388	-3.36207482135086
C	1.16600082901929	-3.57037056093054	-1.16792269719722
H	1.26078452972477	-2.98105457935359	-0.24618607232363
H	0.62262154549609	-4.50308256038184	-0.93457253453107
H	2.18250780499082	-3.84383548570258	-1.50216920752125

C	1.21370270507609	-1.49340024430199	-2.64316394546450
H	2.27102645679277	-1.72953202720957	-2.85271802025176
H	0.78463444128026	-1.01151159132918	-3.53892727652792
H	1.17996835358263	-0.76449447220005	-1.82524139564907
C	0.55363436165240	2.11781834599144	2.16770141150870
H	0.78621894544037	2.58872090728640	1.20086864004202
H	1.24644580923198	2.53827250770943	2.91700726782438
H	0.77170689911483	1.03911237488266	2.10199471378462
C	-1.07145481923073	1.81655587514163	4.05141621859074
H	-0.31583471188236	2.26062337319366	4.72385009765169
H	-2.06875424025020	2.04536158342596	4.46241409532991
H	-0.94341219920785	0.72032638730490	4.06766492262086
C	-1.07130059174080	3.93168805423376	2.66882244768079
H	-1.00939627093947	4.38326761091467	1.66484530428364
H	-2.02575062118513	4.23960677325910	3.12528885785690
H	-0.26556950847712	4.36581128097556	3.28586053844567
C	1.07105130615032	-3.93090883189464	2.67009251110527
H	0.26526995867660	-4.36498518858672	3.28709776098379
H	1.00938662062378	-4.38274992568683	1.66621719327533
H	2.02546360135517	-4.23857995438062	3.12680745559559
C	1.07071216166978	-1.81543800234963	4.05214616292926
H	0.94251553986520	-0.71922207610445	4.06809965161268
H	0.31505263541909	-2.25944172112747	4.72457803430275
H	2.06798391494393	-2.04400470866572	4.46334658574688
C	-0.55404607094846	-2.11740818080270	2.16827431743055
H	-1.24690202335707	-2.53776624046349	2.91759373365145
H	-0.77226119128353	-1.03875467238954	2.10226063759950
H	-0.78642151348074	-2.58859544918378	1.20153483341685
C	-1.21310431631022	1.49260717493716	-2.64360908335791
H	-1.17947053424606	0.76404038105447	-1.82536950845673
H	-2.27040805896715	1.72853935135574	-2.85348730387439
H	-0.78379422912205	1.01039114102190	-3.53907979245712
C	-1.16593225906352	3.57015481819411	-1.16918553499296
H	-0.62270517363615	4.50301586198870	-0.93607781367319
H	-2.18240175855873	3.84337707635168	-1.50374471470815
H	-1.26083935658358	2.98117665920446	-0.24724393640187
C	-0.43484975904479	3.66729172729930	-3.55408501412826
H	-0.05739540870518	4.68672288552853	-3.36356209049278
H	0.15098080400450	3.21941607598853	-4.37537995011949
H	-1.47486662113478	3.77474153098256	-3.90733194250161

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Bis-tmbp reduced

Cu	8.23783355462594	1.68526855754689	3.09630472796371
N	6.73844772658384	2.61372536140419	2.15807986458879
N	6.71003136608278	0.76851401568506	4.03122634074636
C	6.85242401183025	3.56526674149755	1.19081447934778
C	5.72331970391070	4.14779642381076	0.60241037071846
C	4.42616830226228	3.76219964647974	0.99830521354534
C	4.32990168874346	2.78055517177138	1.99608724857155
C	5.49111209391207	2.22379052024360	2.55835535860090
C	5.47370230912654	1.18344696154557	3.61534449037526
C	4.29576276162439	0.65087027430893	4.16248078892840
C	4.35962007545319	-0.33305184726430	5.16271273058674
C	5.64208329022004	-0.74370644632065	5.57370682323900
C	6.79183908622123	-0.18409583240539	4.99878223509397
C	8.25307075235953	3.95179909685798	0.79360322285552
C	3.20133681729022	4.38257046206610	0.37255048899102
C	3.11362894658928	-0.92618007196405	5.77344960469217
C	8.17544850300613	-0.60945025097212	5.42168315520213
H	5.85776713955240	4.90954290146881	-0.17242367671506
H	3.31866365941620	0.99736264740537	3.81544714291389
H	5.75248854158520	-1.50815225306297	6.35042275430988
H	3.18418033309765	5.47515804712725	0.53566578702015
H	2.27232617741873	3.96142251490300	0.78880120548458
H	3.19034473538616	4.22148525570024	-0.72031863780164
H	2.19926766287318	-0.49794856113040	5.33274290155698
H	3.08354052337651	-0.74733669317684	6.86322847136145
H	3.08336088907251	-2.02072104348696	5.62710096646296
H	8.33561212592877	-0.44202304688762	6.50124694219654

H	8.92193989274669	-0.02945112884156	4.85727120183989
H	8.34172054775224	-1.68402737698741	5.22856183783059
N	9.75274553668683	2.63581265915207	3.99924154750853
N	9.74709979370738	0.75893208451783	2.15910652379998
C	9.65938019125309	3.60148913245819	4.95380595787387
C	10.99416677722425	2.25320518165274	3.56715326008921
C	10.99101186206611	1.19353180826306	2.53057254580420
C	9.64804976580008	-0.21566903346662	1.21426591546507
C	10.80105611684675	4.20734269104923	5.49654632238771
C	8.27130820367341	3.98582103178448	5.40036896729815
C	12.16437266390902	2.83260217538400	4.08277044719808
C	12.15806456780387	0.65981178113927	1.96129994543220
C	10.78636089266212	-0.77639842608333	0.61852002004056
C	8.25746792704379	-0.66506949555315	0.84248156639067
C	12.08817824147496	3.83137847993288	5.06696206635119
H	10.68059343576830	4.98048900942169	6.26306659132137
C	12.07595228196609	-0.34511141893309	0.98383655974738
H	13.14108655245112	1.02182337442041	2.27401746501600
H	8.06624851045651	-0.53462204919469	-0.23709980334852
H	7.52292895601179	-0.07236566951997	1.40897215291742
H	8.10554784447561	-1.73392024073024	1.07531083946739
C	13.32561520155921	4.47564686686543	5.64211758623024
C	13.30990182574897	-0.93889073688558	0.34981485872970
H	13.37786331316078	4.32659019003869	6.73548742900689
H	13.32185081646322	5.56640810712828	5.46692336748718
H	14.24511446426385	4.06247699671591	5.19771395211959
H	14.23244297186485	-0.50306339790130	0.76530457699766
H	13.31406604956812	-0.76927881788571	-0.74191863033173
H	13.34801202228012	-2.03195026208907	0.50467048172750
H	8.25162764983602	4.72053767872186	0.00530336401783
H	8.80990315496902	3.07323648659785	0.42262560123236
H	8.81080859442585	4.34475248792954	1.66204282378817
H	3.34212531688895	2.45321212644849	2.33121172933159
H	7.53396620872841	3.39417072769317	4.83643957847799
H	8.07478350385330	5.05863686905518	5.22779203424124
H	8.12935351216713	3.79613793807005	6.47896001024832
H	13.14520993462312	2.51135047348050	3.72230261342385
H	10.66128212026980	-1.55859685700019	-0.13801430799616

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Bis-tmbp oxidized

Cu	8.26010696456964	1.71971950162364	3.06605213129198
N	7.26470998290047	1.15867277416863	1.43792520331320
N	9.71451099951202	2.08769431134806	1.75829651537502
C	5.94287412470244	0.83992132735752	1.37877252938949
C	5.31886223477849	0.63036611520455	0.13875181585168
C	6.02941824942291	0.76626292907082	-1.06867415831165
C	7.38524094482010	1.13757653220071	-0.97194387109729
C	9.7652924462056	1.33102505201939	0.28139791963019
C	3.98546079341424	1.74686708309679	0.47391265968534
C	10.33521321420312	1.77851363313469	-0.55339175559577
C	11.66305183184926	2.16383555923784	-0.28243930702714
C	11.97579452283899	2.47273013522600	1.05502647701160
C	10.99923915138275	2.42050485253820	2.06198762498518
C	5.17174987473206	0.73077841098758	2.66926715754278
C	5.36095942721850	0.56853928555110	-2.40221549875016
C	12.69865852635622	2.24153080394341	-1.37107637074100
C	11.34563289069150	2.69441077071216	3.50276554845562
H	4.25741377478559	0.36510125212819	0.12309062685387
H	10.05743450950381	1.48135812566437	-1.56773126932904
H	12.99860798743071	2.74798144109190	1.32915001565665
H	4.56732701041107	-0.19401329583955	-2.34793603746968
H	6.08150809329140	0.27519739935391	-3.18210652659401
H	4.88394719822018	1.51144042421854	-2.73095352533960
H	12.44569725988342	1.59313753833380	-2.22484879459302
H	13.69857615769762	1.96463709992828	-0.99949407575115
H	12.76986649559657	3.27790314148928	-1.75251218927592
H	12.40797247498042	2.96101519363172	3.60515780980293
H	11.16369737827070	1.80263724183811	4.12940340959695
H	10.74437403176605	3.51943482237262	3.91892232386378

N	7.93533542784512	0.49157462831534	4.59538031035103
N	8.10623055671987	3.12347330119957	4.47081681479194
C	8.02681234546611	-0.8655557497857	4.56392021136907
C	7.81956163615602	1.13875224058765	5.79647265433988
C	7.80480335330045	2.61742585789389	5.70786510783759
C	8.05186499946336	4.46674615436511	4.25992590643085
C	7.94532450487645	-1.61047933669129	5.75171834494421
C	8.21769292667261	-1.54423358723821	3.23151037692390
C	7.74202342204358	0.42953266429026	6.99967307888082
C	7.48682508854378	3.45748115461701	6.77986615852335
C	7.74198768769305	5.34075170439679	5.31507553622792
C	8.32790369015779	4.99169637048021	2.87414060608670
C	7.79077463530466	-0.97933427016352	6.99953138332686
H	8.01294906385172	-2.70114038446209	5.69325248241613
C	7.46622233133772	4.85660217291144	6.60655573520802
H	7.22562078246191	3.03174880022826	7.75201497414819
H	7.82715857214277	5.95974906532879	2.71862963166094
H	7.97724226337444	4.28960216117865	2.10141897870221
H	9.40946080985549	5.15405733774220	2.71406759303752
C	7.72716669911298	-1.76731269928093	8.27998143439135
C	7.16084816564757	5.78506590810003	7.75042619899588
H	7.30346609208533	-2.77121217889283	8.11799612292774
H	7.12988725698827	-1.25036561801443	9.04818193111218
H	8.74488613231855	-1.90433139998802	8.69247863487436
H	6.48489706007135	5.31912325287250	8.48552039002540
H	6.70958775122186	6.72725339001848	7.40110270586619
H	8.09431188399244	6.04701397905111	8.28407824725621
H	4.09074838493405	0.67412240274419	2.47242713283668
H	5.35401992212127	1.60295726496440	3.32005491740004
H	5.45576514969098	-0.17187254375357	3.23781499800720
H	7.96632717291125	1.29550563555000	-1.88399248041196
H	8.87419064183669	-0.95462488563833	2.57162751415686
H	7.25499910222246	-1.68184341478147	2.70699093354620
H	8.66424282377229	-2.54153447685553	3.36381580728982
H	7.66658153835343	0.96533701840884	7.94936344011871
H	7.70686477560144	6.41564844386184	5.11292979796909

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Bis-tmbp triplet

Cu	8.25320972924315	1.71333807616602	3.07194617159115
N	6.78075425614893	2.83236047997121	2.38084588266010
N	6.77747736142330	0.59795210913333	3.76111582860048
C	6.90048190131752	3.88029848210990	1.51237424093868
C	5.77301708027856	4.46727963221496	0.93605683949943
C	4.47056398168474	3.97541297408540	1.21368162168038
C	4.37469107178728	2.87031983046683	2.06215776474791
C	5.52999011449423	2.30120267045590	2.63662252846152
C	5.52808092330455	1.13023899150882	3.50152586670700
C	4.37053278899382	0.56186348031108	4.07227687730188
C	4.46293694635883	-0.54369247287474	4.92048172969265
C	5.76413600297961	-1.03681263629504	5.20202880689918
C	6.89385628655922	-0.45020106914745	4.62982839152582
C	8.29025138680166	4.36748174902822	1.18417849635442
C	3.25517226794679	4.61230552438689	0.58938939151833
C	3.24512506584167	-1.18009208364958	5.54054348109087
C	8.28254408572950	-0.93616426968728	4.96408420417636
H	5.90753001492483	5.31069814341490	0.25198749284007
H	3.39316850226855	1.00936093653672	3.87092598871833
H	5.89578366480135	-1.88061769119556	5.88616172213858
H	3.32763084364199	4.61141182182508	-0.51330342722266
H	3.15917277015421	5.66834983586595	0.90165014577280
H	2.32819964834449	4.08841733607863	0.87198791533733
H	2.31954279768525	-0.65455619109206	5.25645084370134
H	3.31474214780199	-1.18123453128994	6.64341248444529
H	3.14861121062460	-2.23547319071584	5.22617728320684
H	8.25040693884319	-1.67312205957300	5.78105110021333
H	8.92780766886394	-0.09749790987975	5.27952762279317
H	8.77386871314108	-1.40966283273560	4.09707145480436
N	9.72814104428318	2.82149955085511	3.77506414342740
N	9.72647454398141	0.60305652159783	2.36915255584969

C	9.61073204731725	3.85916276563178	4.65606877710853
C	10.97780152837841	2.29214276878866	3.51084975770293
C	10.97687976891042	1.13161483186819	2.63197365434479
C	9.60773951284437	-0.43469036607219	1.48832087865923
C	10.73971542292201	4.43816627581410	5.23745340756892
C	8.22185232400952	4.34366753545894	4.99187947169037
C	12.13458988780123	2.85318920200774	4.09018902987301
C	12.13271160011042	0.57009914328821	2.05122924406104
C	10.73581162352714	-1.01419175204358	0.90564109853045
C	8.21841822542441	-0.9189555788494	1.15421928695826
C	12.04117771859792	3.94828487314413	4.95180783166773
H	10.60721646362358	5.27352110089926	5.93173059959548
C	12.03783192066199	-0.52489211765098	1.18962565186003
H	13.11065954500103	1.01500200216001	2.25545751342487
H	8.24563774412277	-1.63027185326503	0.31467618614486
H	7.56404537238929	-0.07525972877258	0.87352164128343
H	7.74044063652435	-1.42311197795040	2.01165987570482
C	13.25825963619999	4.57667354428675	5.58141301871929
C	13.25386232631193	-1.15382714913383	0.55856184738559
H	13.18692267596434	4.56465166621632	6.68409742429503
H	13.35570370223983	5.63569415563722	5.27983909951618
H	14.18407238481417	4.05419879836420	5.29248261939434
H	14.18012465555725	-0.63091176171691	0.84524811679228
H	13.18053591680992	-1.14310388541009	-0.54399905882502
H	13.35200531515119	-2.21248472931652	0.86120711981277
H	8.26302647683558	5.09035566561570	0.35454882536631
H	8.94357012020114	3.52716511246863	0.89118707264143
H	8.76907782275367	4.85928261401806	2.04823376631203
H	3.39638069529573	2.42363791781421	2.26070616497467
H	7.56696106579245	3.49983219732721	5.27083735053487
H	7.74395024688169	4.85062813692177	4.13607972901641
H	8.25024845098550	5.05276300593627	5.83329511190178
H	13.11211444585249	2.40785979252896	3.88485645808941
H	10.60213095993350	-1.84962343485625	0.21168597842189

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CuCl reduced

Cu	0.00000002874732	-0.00001688555626	-0.01008154176276
N	-1.49211984917068	-0.94537173270202	-0.94475429578057
N	-1.49547408029064	0.93773430586859	0.93152983666237
N	1.49547256057418	-0.93429924696749	0.93497620803766
N	1.49212137156531	0.94189062802169	-0.94822374971489
C	-1.47343806415900	-1.88978230697707	-1.88552829242749
C	-2.63212805500117	-2.46689496807451	-2.45542911496111
H	-2.53223437571746	-3.23701083625457	-3.22300682765852
C	-3.87554193563537	-2.02985024373028	-2.01475466965475
H	-4.79141027811895	-2.45658528747492	-2.43592838155543
C	-3.95517298386712	-1.02486381182783	-1.01325025775629
C	-5.18713574904239	-0.50287683708063	-0.48786181392621
H	-6.13155732561095	-0.89694990681737	-0.87640720601991
C	-5.18889125635811	0.47242553959168	0.48391858002466
H	-6.13474293919170	0.86066248597854	0.87485802223284
C	-3.95884036159099	1.00194366513706	1.00623402974078
C	-3.88297774254241	2.00723724707658	2.00773391097907
H	-4.80052612093453	2.42813611364119	2.43112841201792
C	-2.64122877263958	2.45181671857034	2.44548512552937
H	-2.54422430451240	3.22236539555548	3.21299199941420
C	-1.48048825499265	1.88183526938224	1.87246372005767
C	-2.72600584317254	0.50084340160161	0.50150705804365
C	-2.72421783013666	-0.51601121099817	-0.51167353231555
C	1.48048501380397	-1.87493681243335	1.87937227487898
C	2.64122456580240	-2.44282096837072	2.45447422888032
H	2.54421877649574	-3.21054848976268	3.22480293286811
C	3.88297428818801	-1.99985513263346	2.01509232707148
H	4.80052195061325	-2.41920202309596	2.44002551515744
C	3.95883870226784	-0.99824274000108	1.00991099598507
C	5.18889051629438	-0.47064547433828	0.48565752125319
H	6.13474155645782	-0.85744600412361	0.87801980601922
C	5.18713656017619	0.50108590467431	-0.48969369663850
H	6.13155879222850	0.89373161358251	-0.87967988875594

C	3.95517465860796	1.02114001156592	-1.01699759656007
C	3.87554533476373	2.02244326141207	-2.02218463859503
H	4.79141437177858	2.44763347878770	-2.44491636825591
C	2.63213223900273	2.45786178826145	-2.46446810164297
H	2.53223993050534	3.22515378818862	-3.23486878868603
C	1.47344128130324	1.88283841086540	-1.89246130344648
C	2.72421868659099	0.51412956687415	-0.51356095838694
C	2.72600501650745	-0.49899596984944	0.50334850637791
Cl	0.10042220310282	-2.42215530653320	-2.42255216957739
Cl	-0.10041793600030	2.41322241460590	-2.43145251171863
C	0.09153489731026	2.42409006751516	2.40615633722791
Cl	-0.09153911500240	-2.41522137315531	2.41505658733758

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CuCl oxidized

Cu	0.00000042135118	0.00000005295956	0.00953726466904
N	-1.50470794228755	1.14079603809953	-0.67775766754361
N	-1.49909728888295	-1.14822192567659	0.69242487701904
N	1.50466122689959	-1.14081273429953	-0.67783992058735
N	1.49914555662914	1.14820606003225	0.69234148227500
C	-1.47150814651697	2.23667327791095	-1.44478508181289
C	-2.64175507487862	2.88792940293163	-1.90960707238668
H	-2.54529770342757	3.78194562273264	-2.52959459493744
C	-3.88107183459208	2.37214307408867	-1.55784780361234
H	-4.79694718908134	2.86911658685158	-1.89374831384672
C	-3.96172851929773	1.18910071663727	-0.77023853854606
C	-5.19182859808665	0.55996961561687	-0.37640403055565
H	-6.13751494894951	1.01396941756013	-0.68763712720526
C	-5.18907814291531	-0.59161245771633	0.38086913479903
H	-6.13264138692543	-1.05164863804962	0.68967140960954
C	-3.95590201796092	-1.21272405458083	0.77797121010444
C	-3.86975247416550	-2.39482787147584	1.56622511206881
H	-4.78334526422548	-2.89730955639441	1.90015813051561
C	-2.62810454490380	-2.90262397843785	1.92159859170893
H	-2.52769677709867	-3.79565280662456	2.54236172928486
C	-1.46099978851648	-2.24418520771876	1.45917167255074
C	-2.72714226235933	-0.61646135153853	0.38136093361416
C	-2.73001906616257	0.60076475680366	-0.37073519908402
C	1.47141036492087	-2.23668899366186	-1.44486616851921
C	2.64162665212223	-2.88796103142670	-1.90974302992134
H	2.54512793205773	-3.78197540546008	-2.52972672995468
C	3.88096699501740	-2.37219251822295	-1.55804087528647
H	4.79681974291356	-2.86917879451910	-1.89398423612934
C	3.96167684179547	-1.18915168358003	-0.77043477476469
C	5.19180383279240	-0.56003763862412	-0.37665702599006
H	6.13746958368221	-1.01405047326251	-0.68793373018583
C	5.18910423578139	0.59154477821932	0.38061584681668
H	6.13268806760175	1.05156815720622	0.68937424206489
C	3.95595504925406	1.21267385207227	0.77777430303514
C	3.86985840100333	2.39477981548683	1.56603088586221
H	4.78347368024642	2.89724925531995	1.89992085111450
C	2.62823401687034	2.90259376635273	1.92146114744709
H	2.52786746215561	3.79562481878149	2.54222770685059
C	1.46109870063752	2.24417051315656	1.45908919573594
C	2.72716879715364	0.61642779264281	0.38122121503957
C	2.7299400491277	-0.60079870370687	-0.37087437601256
Cl	0.09306735109043	-2.86276374634255	1.90694423412784
Cl	-0.09293922245588	2.86277000414042	1.90693353807168
Cl	0.07944949806358	2.86737250072929	-1.88579876106572
Cl	-0.07957647826227	-2.86736790401298	-1.88580742043739

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45

CuCl triplet

Cu	0.00000290919620	-0.00017889823892	-0.00973919768395
N	-1.47982446779440	-1.16068469533099	-0.65992377073837
N	-1.48526222631014	1.15315751046061	0.64588569014794
N	1.48523882701171	-1.15117366454171	0.65005550092339
N	1.47985723072723	1.15797894554249	-0.66402923416687
C	-1.45366576061765	-2.26403931681767	-1.42691207101697
C	-2.60822992648775	-2.92004001701148	-1.88873762043355

H	-2.50439640089315	-3.81849529641760	-2.49966413162665
C	-3.86369984937118	-2.40588472214220	-1.54218685489069
H	-4.77555118335192	-2.91132581145399	-1.87445053923013
C	-3.94736759019054	-1.22326090694764	-0.77219981843372
C	-5.17854303258280	-0.59343123361351	-0.37606744503199
H	-6.12266579801272	-1.05637779074461	-0.68016763165972
C	-5.18118560387635	0.56012561763157	0.37450171823572
H	-6.12741507191108	1.01661346061810	0.68181101355198
C	-3.95305639286724	1.19845576883392	0.76648141102853
C	-3.87532898955378	2.38174891219015	1.53612175760594
H	-4.78975771695015	2.88083436515911	1.87089737425163
C	-2.62241383524972	2.90469382462144	1.87841416146569
H	-2.52282734906997	3.80415709658155	2.48854164611079
C	-1.46484998848014	2.25604867609194	1.41337824392991
C	-2.72351897554049	0.59887050318193	0.36048888453143
C	-2.72067566088428	-0.61505427620539	-0.37027455566176
C	1.46479768870612	-2.25131323161380	1.42148471501660
C	2.62234172417253	-2.89829987756929	1.88887294124968
H	2.52272903369180	-3.79557034503067	2.50221624555355
C	3.87527124436888	-2.37659909396519	1.54473892077577
H	4.78968631577366	-2.87449147424898	1.88132319881922
C	3.95302974704680	-1.19607242034078	0.77086469930592
C	5.18117567323420	-0.55916512149378	0.37662933230919
H	6.12739245663278	-1.01456231711780	0.68559135390518
C	5.17856351598370	0.59169798906264	-0.37806350165119
H	6.12269842833528	1.05354137420975	-0.68379897380939
C	3.94740460901501	1.22012111927869	-0.77647401892731
C	3.86377024952720	2.39998067879350	-1.55069431770500
H	4.7756357078844	2.90421602624805	-1.88474651651370
C	2.60831440116379	2.91290709873134	-1.89911145476586
H	2.50450564901543	3.80916993230289	-2.51325407038575
C	1.45373119807786	2.25857945479469	-1.43496399091778
C	2.72069614022516	0.61337368535030	-0.37240021066240
C	2.72350910959378	-0.59792935066296	0.36270074488475
CI	0.10977918884497	-2.89346738106263	-1.86979418330590
CI	-0.10969325364305	2.88644286914179	-1.88013116700637
CI	0.09552492504646	2.89967411493459	1.84869698423930
CI	-0.09559680554048	-2.89335734318946	1.85907784838290

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97

Bis-bcp reduced

Cu	0.01703463503791	4.07312799408441	6.56925236773806
N	0.84832566510078	2.93089413140916	5.15038823940499
N	-1.01772845995754	4.80068721879085	5.02010186752275
N	-0.82804413248180	3.32269816440348	8.21851579664546
N	1.02863180842338	5.18308958897426	7.90181722898668
C	0.33135490410793	3.17818855740101	3.90120097266315
C	0.73852712675571	2.48407740257505	2.72496898795765
C	1.79042076548470	1.97273042729889	5.27309465082902
C	2.33918687634886	1.72279807470195	6.65375799128915
C	2.25651711925464	1.25098592180817	4.15143043427715
C	1.76809607566004	1.49081112401600	2.86184919651765
C	0.05352826009924	2.78031467471975	1.49707965788903
C	-0.91463001399464	3.75679510864987	1.42848690135391
C	-2.27988954817674	5.56896941640673	2.57638788927786
C	-2.61047790250904	6.14254511162606	3.80977401075541
C	-1.97684303748790	5.74987327255046	5.00999733812484
C	-2.32209645191582	6.38759914022612	6.33071231065292
C	-0.68493006801111	4.19946413878022	3.82972174638709
C	-1.28975253359296	4.52751221942088	2.58175001427931
C	-0.33453321665361	3.88222152633392	9.37071386601579
C	-0.77569585877990	3.51999876207301	10.67770513312727
C	-1.78987634705078	2.38102270722027	8.32462640828313
C	-2.31103664045133	1.79672096161865	7.03772636196167
C	-2.26624841078394	1.95690475498822	9.58325057958250
C	-1.77029655204511	2.48971890429689	10.78087869629801
C	-0.24179496148056	4.24933999862197	11.79529882876449
C	0.72190936000805	5.21820239476075	11.63101442740027
C	2.25758590124867	6.53840816159420	10.09328511314736
C	2.57471743016379	6.81840836700956	8.75895316786249

C	1.95642295001398	6.13814284270554	7.68599662988483
C	2.31809028876900	6.43396730060563	6.25366976407599
C	0.67691597966335	4.89814230179355	9.19923306301824
C	1.24305583254496	5.54938363381363	10.33310581748649
H	3.42980721851477	1.89390513085599	6.69050313796624
H	2.16193808688003	0.68082490197961	6.97503271462558
H	1.84725150363804	2.40377797714997	7.36555307604177
H	3.05018744300298	0.51118180698220	4.29569091539194
H	2.72149776403857	2.48024939052186	0.48308378669531
H	3.69427526583789	1.18193934876541	-1.40227283636904
H	3.87431282457844	-1.30980777540196	-1.25439171526473
H	3.07120692707961	-2.49393461837829	0.79983553565433
H	2.08072200539564	-1.19804120554772	2.68216725470987
H	0.29563490517830	2.19328445611635	0.60739751068093
H	-1.43552118167848	3.93848927800286	0.48497422027883
H	-4.94462924566603	5.89745182636316	2.16979343198584
H	-6.07655381664564	6.77285126185152	0.13165748246292
H	-4.72674979385909	7.42095904565538	-1.87447462076911
H	-2.23407713159110	7.20238986674255	-1.81792704605160
H	-1.09947524224286	6.34541289028116	0.22312815014898
H	-3.35327565011018	6.94555180090502	3.84531551758349
H	-1.71181625622423	5.92550354658500	7.12261958632700
H	-3.39035652754730	6.25274490316427	6.57717042832706
H	-2.12590979642329	7.47457601224815	6.31656843957695
H	-3.08362171199999	1.03401276804830	7.22086843100719
H	-1.49218160336701	1.33256255982594	6.45977693050251
H	-2.74555650116721	2.58763424615012	6.40062227743887
H	-3.01815599619753	1.16325589040313	9.62185815245101
H	-4.36625424795876	2.18035014391690	11.51183424650697
H	-5.24566669321027	1.25958372898652	13.65170765474637
H	-3.66430141473928	0.53647656823255	15.45244197712511
H	-1.19536888255833	0.72475682970890	15.08663235770940
H	-0.31372130730089	1.62668718408296	12.94252108992180
H	-0.63687512242185	4.04169332933965	12.79296312615984
H	1.08694057703534	5.77291389055554	12.49916773619215
H	2.62422328146301	9.21817952481751	10.32100979295623
H	3.86889912389144	10.43883355882224	12.09963884686689
H	4.91965957787744	9.17702341529762	13.98913634796016
H	4.73109473857711	6.68287014108929	14.07411871051302
H	3.50335094093819	5.45965831951622	12.28889205946883
H	3.35015280737561	7.55805888329786	8.53583488035896
H	1.76980141887273	5.74589307483142	5.59116518449599
H	3.40189586828364	6.31491995286778	6.07885140907446
H	2.05596968286493	7.47200208134571	5.98011643677967
C	2.31776786065615	0.73039366528197	1.71094563397287
C	2.77291246013813	1.38817181078799	0.54432188380063
C	3.33304064218493	0.65687184328227	-0.51210956348219
C	3.44073222219811	-0.74045326731165	-0.42612339779367
C	2.99403030094897	-1.40428976712143	0.72779355073342
C	2.44347841948025	-0.67558655364534	1.79031849533083
C	-2.94382868365828	6.04701027393261	1.33701883585164
C	-4.34949607708339	6.19335893601532	1.29907363853044
C	-4.98599991960880	6.67876155323318	0.14909745028158
C	-4.22914626726577	7.03851100179813	-0.97763696198206
C	-2.83130797714927	6.90930411365273	-0.94846330770366
C	-2.19200667535845	6.41427100099326	0.19637864244950
C	-2.27873618567020	1.98144687610944	12.07998597220020
C	-3.67069931807902	1.85125268653628	12.29144035776009
C	-4.16464550747671	1.34048878733871	13.49899709996729
C	-3.27761971340485	0.93862156421435	14.51064672896147
C	-1.89271899999098	1.05089357678746	14.30823398511612
C	-1.39507306086396	1.57116593159609	13.10571675137892
C	2.96365047600042	7.25466414353588	11.18596187265449
C	3.09476712345857	8.66155145365847	11.13872189029001
C	3.78866651199885	9.34792875829483	12.14399419653151
C	4.37473703213247	8.64046863147244	13.20595629863401
C	4.26279360879013	7.24179938157573	13.25749529427348
C	3.56040104589605	6.55277335672350	12.25930657454444

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Bis-bcp oxidized

Cu	-0.03183028914542	4.01024005180642	6.57996058807218
N	0.59604633224963	2.71850965016153	5.19179578854363
N	-0.87206136760627	4.92437320299164	5.01436386158422
N	-0.67579603456919	3.11007273268278	8.24494035659911
N	0.78477506247175	5.29663214639696	7.87079067942574
C	0.19416105688263	3.08130374032301	3.92871361081045
C	0.53372828826704	2.34761349391623	2.75715876911046
C	1.38716602509203	1.63387802914095	5.34046019503608
C	1.84957712675459	1.25883345999784	6.72380660173695
C	1.79821823879477	0.88351733355857	4.21712161227533
C	1.40387435755458	1.20804291322490	2.91202117795748
C	-0.05315125250563	2.75961493910103	1.51376053789510
C	-0.85400424906496	3.87811077795428	1.42914979831299
C	-1.94278886925259	5.88344047520407	2.55425584261612
C	-2.23970339088070	6.47186194754242	3.79050432874388
C	-1.69477650400259	5.99450995069595	5.00318756697558
C	-2.00286835211743	6.68521457643725	6.30591755945555
C	-0.61224390633476	4.27033781937819	3.83365506812010
C	-1.12037023355243	4.69877232229766	2.57524326727995
C	-0.26023767888414	3.76574782570244	9.37973472165905
C	-0.60881144235026	3.34841294020424	10.69478910591645
C	-1.50159702980823	2.04950279618884	8.36729052026360
C	-1.98558802066584	1.35913911542631	7.11910173400368
C	-1.89112704235663	1.58195328266035	9.64234613109677
C	-1.43286858875213	2.17187671595346	10.82723803645724
C	-0.19134284890042	4.17154907694218	11.79303415490287
C	0.60250711330389	5.28180139278888	11.60124194912127
C	1.88459064675184	6.81243828930243	10.02070746376540
C	2.11722586987182	7.12432688882001	8.67440652250427
C	1.56326616075868	6.37065367046753	7.61656020578747
C	1.85775386682210	6.72941669474672	6.18379226598078
C	0.54024959262696	4.94512638225943	9.17654619195024
C	1.03140252484072	5.68175334215386	10.29129159212546
H	2.91208883068644	0.96475783072752	6.71268952895186
H	1.28059684509879	0.39477045381842	7.11310088113622
H	1.72280072757936	2.09730140366157	7.42483166025175
H	2.48479739709826	0.04700637045193	4.37574021918296
H	2.49449359395883	2.10802072099434	0.55519307013489
H	3.36884339146549	0.71983927565444	-1.31090117649729
H	3.29578408969556	-1.77622329775313	-1.16420137810647
H	2.34423877986513	-2.87910917408549	0.87037158682473
H	1.45619736245283	-1.49864266029726	2.73941908150565
H	0.11775891935695	2.14719286972287	0.62546881712941
H	-1.32555483039487	4.13738459042989	0.47815504583337
H	-4.48407635334581	6.73275271451571	2.11260149813264
H	-5.38345362014245	7.80545109856456	0.05703060760836
H	-3.89757481548913	8.16921479926671	-1.92322199270587
H	-1.49877527074718	7.46589194429836	-1.82971848523719
H	-0.58651159177166	6.40369827070049	0.22350186955873
H	-2.87365437291997	7.36290556552690	3.82289273415854
H	-1.78815493805573	6.02929711519982	7.16279227720822
H	-3.06294869828599	6.98489135937615	6.34681178153779
H	-1.40264369734518	7.60639988686436	6.42013446284131
H	-3.05823373936518	1.11670085962786	7.20057994167475
H	-1.45173851613599	0.40487991622713	6.95781006235890
H	-1.83377626880309	1.99203700055956	6.23226599227980
H	-2.53248575117917	0.69719584997012	9.69547612544938
H	-3.90368638393865	1.34759796699940	11.59574665812739
H	-4.54043307966622	0.29064116028506	13.75509270516031
H	-2.81559599876229	-0.07862131721753	15.52990214019358
H	-0.44291482322878	0.60319787499573	15.12578186790907
H	0.20683796532086	1.64912722778693	12.96691970424283
H	-0.54071569134221	3.92145550853600	12.79771210955200
H	0.88965882430707	5.89656650836110	12.45734242993116
H	1.97432607409228	9.51946801377817	10.16500790513012
H	3.09537304201111	10.90651381588555	11.89921363611464
H	4.28584420548854	9.81093802784006	13.80801633500878
H	4.36238661987759	7.31545970222562	13.96300082949730
H	3.25497221758076	5.92065350725490	12.23020095401220

H	2.78669062805022	7.95278018088654	8.42581822714935
H	1.63418891973479	5.88839183415290	5.51060550883899
H	2.91797171703409	7.00665992931845	6.06253397843440
H	1.25860873328887	7.59980856222850	5.85907801021648
C	1.89279615687252	0.40275168230093	1.77308286933282
C	2.42815517327682	1.01674705236697	0.61333124612485
C	2.93708932804955	0.23426242416389	-0.43043796939256
C	2.90471718840866	-1.16747376702955	-0.34329590255110
C	2.37580035694594	-1.78752184809902	0.80177622622611
C	1.88529422336018	-1.01099341868411	1.85757806913354
C	-2.47534864542969	6.47701844081219	1.31036143306591
C	-3.82493634523834	6.90601117818640	1.25533513001859
C	-4.33367620108152	7.49933395499042	0.09496593485405
C	-3.50008324669024	7.69754696511790	-1.01937991215983
C	-2.15462165572935	7.29398529531497	-0.97084590623113
C	-1.64484887981566	6.68051588100267	0.17946743223542
C	-1.80651732874245	1.58859431109718	12.13227071619759
C	-3.14140031287293	1.17179926971695	12.36217250895532
C	-3.50174614715780	0.58738910122346	13.58116733514798
C	-2.5358868707555	0.38612481638572	14.58022384723663
C	-1.20221145074566	0.77760288501553	14.35741108429718
C	-0.83933703539885	1.38206952963104	13.14813353481310
C	2.51656647476876	7.62179865819082	11.08394102111428
C	2.50672025472993	9.03492059781199	10.99044815652828
C	3.12898287173070	9.81521695038395	11.97142137500111
C	3.79244201183171	9.19932018495904	13.04652044999718
C	3.82742446805650	7.79800029190777	13.13936966192974
C	3.18832182252907	7.01194831946423	12.17269664130837

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Bis-bcp triplet

Cu	-0.00703840780578	4.02259092497044	6.57778314619726
N	0.56795094205184	2.71037142031655	5.21474502910788
N	-0.78477432546226	4.96958199147951	5.02658910975327
N	-0.58091250168277	3.07357765197545	8.21506660603689
N	0.74101194387228	5.33019186360099	7.85699954315172
C	0.19544784069236	3.09030990769320	3.93765695211318
C	0.53616678894166	2.34348778310597	2.77012358678538
C	1.37771362806279	1.63049274637990	5.36236415007540
C	1.85544333531996	1.28170111555175	6.74976985843970
C	1.78367809622032	0.87975858586820	4.24671852390987
C	1.37849989080314	1.19795007731095	2.93227716868866
C	-0.04371763934555	2.77048574416749	1.52488634778176
C	-0.83190754908542	3.89582242036868	1.44062989499360
C	-1.89571038688101	5.91033184415600	2.57105073148156
C	-2.17847204004990	6.50798398352410	3.81859633902105
C	-1.62116707623494	6.03965706386368	5.01949801310413
C	-1.92557907812784	6.71481400071884	6.33334453867196
C	-0.57259889942667	4.28807133132836	3.84091925481359
C	-1.09193210777594	4.72574760583194	2.58613931834956
C	-0.21534787445891	3.75202823105621	9.36446725826232
C	-0.57054864230119	3.31412229502642	10.67514631353886
C	-1.41279256544499	2.00586470794417	8.32824376621245
C	-1.89272205516148	1.33978782287363	7.06299759632589
C	-1.81061560848203	1.53601681473235	9.59040235998651
C	-1.36874051013160	2.13153731981996	10.79204897799498
C	-0.16221500927555	4.14162805059841	11.77848483162392
C	0.61237768197846	5.26459318308338	11.59473304852185
C	1.84465148812294	6.83616091439932	10.01721123782270
C	2.07690222137238	7.15578420436625	8.66185706306675
C	1.52760674072799	6.40826380968183	7.60715821247622
C	1.82177256222397	6.75896563498155	6.17000974523195
C	0.53708914725215	4.94793776298888	9.17104803771940
C	1.02765289584016	5.69226512554328	10.28559219820557
H	2.72572474392629	0.60884094975358	6.70459009843132
H	1.07150959782074	0.77764147873085	7.34241729391960
H	2.14165756208455	2.19104055108753	7.30539992267394
H	2.46401171487308	0.03850109365106	4.40583413251408
H	2.50322684376938	2.0255279765713	0.56422954036259
H	3.31880644667631	0.58797538019687	-1.29298449197289

H	3.16463061273239	-1.90413719488197	-1.11777340301733
H	2.18286815090711	-2.94610964738317	0.93625969870778
H	1.34297564262914	-1.50918996922217	2.78690648625320
H	0.12167038163449	2.15785277061500	0.63510744455261
H	-1.29579960656328	4.16181052306143	0.48738529913447
H	-4.44030270194223	6.76081002202152	2.14908970659572
H	-5.36344420843503	7.83763320031507	0.10535021598858
H	-3.90242470872972	8.19806592750844	-1.89577453626200
H	-1.50249977211513	7.48999430259018	-1.82420401283968
H	-0.56942577327482	6.43737218752826	0.22564772393265
H	-2.80962155130656	7.40064206341902	3.85307809967213
H	-2.08996580265498	5.96785134732213	7.12859643073244
H	-2.82556763318036	7.34349537625138	6.24934888240231
H	-1.09498860239413	7.36151927362738	6.66814740289218
H	-2.73909653817616	0.66777172364360	7.27292913107619
H	-1.09862416116749	0.74265356864975	6.58111286628699
H	-2.21816963805185	2.09293093443564	6.32461727725678
H	-2.44312960000569	0.64490647368845	9.63639254791808
H	-3.84137542476231	1.28930047528811	11.53411523963277
H	-4.50089324826161	0.21530464161561	13.67909003117096
H	-2.79838294351387	-0.15082844651351	15.47805289256128
H	-0.42447441476232	0.54830476747601	15.10141674408321
H	0.24394438317507	1.59799880991247	12.94901501121290
H	-0.49991548426142	3.87580390071775	12.78343452226548
H	0.89305841947401	5.87497520719832	12.4567135752146
H	1.83593735963710	9.54329376788559	10.17041341040642
H	2.91426581258969	10.97426375242674	11.89801343015393
H	4.15204978243912	9.92558705565220	13.80501887256865
H	4.31983780628209	7.43274098241485	13.95506514811047
H	3.26495989521501	6.00103107778951	12.21765532954996
H	2.73296477414539	7.99584369105386	8.41738036518800
H	0.97015188619060	7.27010943146718	5.68681345601477
H	2.02669199223206	5.85012162125321	5.57885696229137
H	2.69464955033870	7.42662193844409	6.10282456578310
C	1.84430492118929	0.36152485262077	1.80144522374928
C	2.40294183416451	0.93756364289402	0.63509940354602
C	2.87646382380679	0.12594836101206	-0.40445161173838
C	2.79731965360401	-1.27227468376328	-0.30293481933806
C	2.25066572375746	-1.85674207613413	0.85129808424950
C	1.78546127913645	-1.04917778180591	1.89666922567262
C	-2.44222151801516	6.50746979968252	1.33094885056359
C	-3.79163433460969	6.93246234431007	1.28331816983290
C	-4.31312221390162	7.52977224299889	0.12904534465107
C	-3.49497462123734	7.72756158092362	-0.99537507283103
C	-2.15069116820011	7.32317172164380	-0.95780471458542
C	-1.62766321849773	6.71633563251729	0.19164704183848
C	-1.75457752731030	1.53522329958209	12.09145362221465
C	-3.08850438147340	1.11504859744381	12.31041085095703
C	-3.46100864317341	0.51931494547463	13.52179202061775
C	-2.50710683757563	0.31833856607036	14.53298286428446
C	-1.17705017438536	0.71774715856726	14.32453798861256
C	-0.80235473457182	1.32298242956456	13.11773618445720
C	2.45551239034457	7.66924469608823	11.07937788508578
C	2.38910805646960	9.08029108577121	10.99477061986954
C	2.98908551098209	9.88454325340827	11.97180923622333
C	3.67967848025334	9.29631931546201	13.04408425266907
C	3.76695456490850	7.89768920774548	13.13240207039492
C	3.15955037577306	7.08940786499278	12.16216460661090

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Bis-dbdmp reduced

Cu	0.00304795914702	-0.00123715560225	0.00509226521446
N	-1.50188415455181	0.55044996178089	-1.20999409683011
N	-1.51348445210252	-0.51685841190704	1.22136213495161
N	1.49888378225030	-1.23535980161520	-0.52884523460873
N	1.52872934064175	1.19578927173107	0.53860459565630
C	-1.44810872451141	1.09521308504695	-2.44218697954673
C	-2.62870017546263	1.44272665339529	-3.14445300881923
C	-3.89687325907929	1.22773897754833	-2.60784203423420
C	-5.14273784823871	1.60318668224558	-3.37027491551917

C	-3.96460448877540	0.63695900366442	-1.30422549522283
C	-5.19296608909315	0.34537780177817	-0.61970749356357
H	-6.14224368965060	0.57968611075293	-1.10971125078277
C	-5.19916998102460	-0.22297564733070	0.63483585167073
H	-6.15331387187412	-0.43436677237455	1.12581196716599
C	-3.97749173700865	-0.54404912155791	1.31810431787927
C	-3.92270414104786	-1.13629316379133	2.62166153307530
C	-5.17646890383629	-1.48144108163364	3.38546162073266
C	-2.65953345160373	-1.38180485695901	3.15695640711892
C	-1.47163376240508	-1.06277594256908	2.45350276320203
C	-2.74389675071950	-0.26120767059074	0.66495344945108
C	-2.73751718193807	0.32450612485367	-0.65232615845172
C	1.43598791120547	-2.46676342615735	-1.07440986206681
C	2.61163003249615	-3.18446892778379	-1.40683496798305
C	3.88386530980197	-2.66454213293049	-1.17552034116166
C	5.12433804862127	-3.44334579491205	-1.53486091217330
C	3.96108445961527	-1.36186500283498	-0.58383850474619
C	5.19447925355855	-0.69350994741467	-0.27644296598454
H	6.14017040992996	-1.19597970000473	-0.49854701888108
C	5.20985814991204	0.56089859424678	0.29203118043677
H	6.16757109407970	1.03930860511188	0.51572389196355
C	3.99323010856602	1.26018683365952	0.59740381093758
C	3.94795050518842	2.56441748407038	1.18897117760531
C	5.20709591118194	3.31166053698661	1.55039957601427
C	2.68886832911887	3.11632762118236	1.41818161010967
C	1.49603191965097	2.42849694171588	1.08387759873879
C	2.75490139111023	0.62323887199759	0.29873616356741
C	2.73874080452299	-0.69391066764884	-0.28708589905515
C	0.06488390371861	-3.05838022337901	-1.29610439412047
H	-0.67232834445975	-2.25532946787817	-1.11575708164010
H	-0.03699184062489	-3.37314393827678	-2.35317105197199
C	0.13986213162355	3.05456551382254	1.30287211883984
H	-0.61697876647582	2.27045630516558	1.12048008406264
H	0.04352848122902	3.37138644156691	2.35984367471329
C	-0.11035796250726	-1.29945285555200	3.06178089851513
H	0.63849496648596	-1.12788170374871	2.26762799602164
H	-0.02410705513722	-2.35735497210281	3.37837790343393
C	-0.08204674764577	1.29933680814412	-3.05155918580185
H	0.66308169359548	1.10826300160023	-2.25834376550285
H	0.02982959254462	2.35534117974207	-3.36652168881999
C	-0.13429505607633	4.27081495009843	0.38686943584929
H	-0.05409040717866	3.95146430458689	-0.67037970005850
H	0.65211245607659	5.03571558722961	0.53853047979192
C	-1.51540649589904	4.89984757854779	0.63745917487307
H	-1.58690632868875	5.20807645655888	1.69898090266877
H	-2.29770974258855	4.13007064635872	0.48857055017778
C	-1.79563465471880	6.10687921744423	-0.26982832660442
H	-1.76448116686909	5.82299506429623	-1.33730724631323
H	-2.79104491375232	6.53753932488040	-0.06662085155101
H	-1.04855219910242	6.90598407249138	-0.11584356416092
C	0.19207503216456	-0.38626310429337	4.27345232030451
H	0.12240241165931	0.67171538406477	3.95405383767745
H	-0.58645054309694	-0.52637202731485	5.04856275460134
C	1.57757371299859	-0.65538997548099	4.88494244451853
H	1.63821871670732	-1.71742591712344	5.19372372704535
H	2.35187640039621	-0.51841670793337	4.10493341589758
C	1.88604479635885	0.24936426241475	6.08697926634585
H	2.88400714133421	0.03277708071407	6.50502855713653
H	1.86614795893087	1.31682266043213	5.80200591990390
H	1.14728795649461	0.10683811961159	6.89589024041463
C	0.19684409112858	0.38098368749041	-4.26494449250596
H	0.10177417468049	-0.67549587362721	-3.94712891968809
H	-0.57878001044202	0.54122851566273	-5.03905337767111
C	1.58787243360588	0.61727864516747	-4.87745717277776
H	1.67416542753024	1.67812026521899	-5.18423913003621
H	2.35942408416475	0.45984574030419	-4.09858213870207
C	1.87279520601787	-0.29238988208509	-6.08159466447964
H	2.87531641400890	-0.09948960887658	-6.50033333971205
H	1.82705264944513	-1.35960497167607	-5.79869817271511
H	1.13688485408628	-0.13019780199935	-6.88939646878219

C	-0.24199850171252	-4.26696743964340	-0.38033005466210
H	-0.15725464947242	-3.94907599066518	0.67700411167395
H	0.52576764154884	-5.05113256499389	-0.52917134602361
C	-1.63740792375355	-4.86194989509517	-0.63489770310831
H	-2.40099329934979	-4.07299220846505	-0.48927969762519
H	-1.71302660110320	-5.16935165646968	-1.69637359120887
C	-1.95030083680761	-6.06083243231874	0.27251987865387
H	-1.91560582863946	-5.77677706730912	1.33984408997420
H	-2.95538664161708	-6.46695680455052	0.06644280755931
H	-1.22270159616017	-6.87830392014638	0.12167555564585
H	-4.89145284784669	2.04841027956845	-4.34571048494352
H	-5.75406367906729	2.33492379583376	-2.81139716736347
H	-5.78344183592410	0.72188974361940	-3.55603253769912
H	-5.79543573405570	-0.58486371280438	3.57178893397999
H	-4.93497112760459	-1.93251247569311	4.36068258264867
H	-5.80594767970260	-2.19822725869246	2.82736221732654
H	4.86602022701475	-4.41547119211233	-1.98328788200160
H	5.75108564651794	-3.63736069754206	-0.64534491016304
H	5.75239098117322	-2.89269747799426	-2.25862684588349
H	5.84006690565503	3.48973540421545	0.66195998848641
H	5.81978400168840	2.74535997610624	2.27525861431640
H	4.97264545472719	4.29001919826569	1.99838454144349
H	2.60894797148081	4.11126533188304	1.86923453084263
H	2.50733674682463	-4.17703576572962	-1.85814071401229
H	-2.53170091328834	1.89273302457549	-4.13834725136388
H	-2.57231238992400	-1.83401391225949	4.15075658846879

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Bis-dbdmp oxidized

Cu	0.00017155848230	-0.01230826470072	-0.00063075600891
N	-1.18260449561901	-1.50377955742023	-0.62239404682641
N	1.17711251465840	-1.50819140290033	0.62135765713450
N	1.01400068461743	1.48047638557357	-0.87047273359552
N	-1.00801107594839	1.48495417368540	0.86776604660735
C	-2.32438372068652	-1.43777725573022	-1.33703369936305
C	-2.98024235754085	-2.62756695231084	-1.74937016059269
C	-2.49086956987175	-3.89432457739796	-1.44171964938618
C	-3.22455685725698	-5.13840408685234	-1.86364409088813
C	-1.25325807661666	-3.96071444560307	-0.71421260435078
C	-0.60465401756779	-5.18680109424989	-0.34799438215038
H	-1.06851814549221	-6.13676545149066	-0.62590206461234
C	0.58517487809344	-5.18901593279115	0.34746281919529
H	1.04542717049055	-6.14067619418383	0.62554890721297
C	1.23843988318189	-3.96532945694237	0.71346792418374
C	2.47634994389096	-3.90350524622482	1.44097722537118
C	3.20516591208968	-5.15040201255530	1.86300541254694
C	2.97049092314563	-2.63858409297218	1.74848841941947
C	2.31909022573321	-1.44638718314098	1.33603417471754
C	0.62453798337626	-2.73712348341950	0.34493664287056
C	-0.63468872285524	-2.73478371636138	-0.34589518956803
C	1.95149122713624	1.41153606714765	-1.83788965455582
C	2.47228582897536	2.60015285125474	-2.41327740307430
C	2.06602435288572	3.86778634032630	-2.00436421025624
C	2.66053333863288	5.11081458871957	-2.60894627063534
C	1.04631511651278	3.93673107842603	-0.99398606078735
C	0.50200350924105	5.16294202836107	-0.48533015064984
H	0.88382334057785	6.11289478715842	-0.86832445165244
C	-0.48402202792773	5.16519219804705	0.47778943687525
H	-0.86274889494383	6.11689805159703	0.85950219232169
C	-1.03229391157448	3.94143395744891	0.98809015868652
C	-2.05218730073305	3.87711861667151	1.99857878383181
C	-2.64262666765350	5.12284961533992	2.60158392419907
C	-2.46257327469973	2.61134471433554	2.40916449738410
C	-1.94570692846987	1.42029364736767	1.83527996007006
C	-0.52799018950662	2.71388979931627	0.47893983439321
C	0.53808025221144	2.71149667015890	-0.48317766190082
C	2.42481308431830	0.06005036547419	-2.31312549816471
H	1.81532986314851	-0.72176960694223	-1.82705499314221
H	2.21913306660097	-0.00924635146918	-3.39972073296240
C	-2.42336335217731	0.07093537314587	2.31225095154261

H	-1.81636234219184	-0.71346758400795	1.82721314570396
H	-2.21787392950889	0.00242230244365	3.39893434357782
C	2.86386044893546	-0.10401280036816	1.75021021390559
H	2.43633100431476	0.68444399581147	1.10786174930531
H	3.95934260306935	-0.09174938383847	1.60112536357343
C	-2.86418889938612	-0.09346118875422	-1.75141727474921
H	-2.43459278682030	0.69345092156034	-1.10856610250127
H	-3.95975398458168	-0.07753685155066	-1.60333148619309
C	-3.93037398247862	-0.19854903852695	2.07995702358827
H	-4.15176736225521	-0.14239608406071	0.99692524520322
H	-4.52788101014997	0.60147901402239	2.55674302522509
C	-4.37207993474392	-1.56385405809964	2.63605636827935
H	-4.13659673426716	-1.60822800418982	3.71695131674952
H	-3.77254854218410	-2.36379771965449	2.15806174004354
C	-5.86851129971734	-1.83504448210568	2.42248521430466
H	-6.13282417565399	-1.82784089473756	1.34973515497066
H	-6.15443877611520	-2.81835743419717	2.83143426780917
H	-6.48981398360452	-1.07324028218894	2.92499287857891
C	2.55881934491131	0.21558546601451	3.23965482698961
H	1.46209789582559	0.20954442598045	3.39545490792036
H	2.96586424746593	-0.59015535384148	3.87951380408998
C	3.14473169616041	1.56916465402133	3.67898060668057
H	4.23889641571102	1.56224450224519	3.51151068082511
H	2.73888061288989	2.37100398703826	3.03080160727221
C	2.84970177785528	1.88952416970771	5.15187378702650
H	3.28211480173524	2.86284260566784	5.43769165752679
H	1.76308401229501	1.93430874962490	5.34677440136534
H	3.27938982474997	1.12516030863856	5.82261337862712
C	-2.55672539507018	0.22531480062988	-3.24053998387060
H	-1.45988631032008	0.21563652211614	-3.39533795656480
H	-2.96586592693709	-0.57899165775276	-3.88086836429874
C	-3.13773107544317	1.58088648244478	-3.68023565040395
H	-4.23206452986732	1.57758928639434	-3.51376508735835
H	-2.72981736521827	2.38129818988242	-3.03158925997890
C	-2.84030603562419	1.90044410904626	-5.15282272815692
H	-3.26918403490229	2.87524916616411	-5.43890135141595
H	-1.75336796794196	1.94159067089198	-5.34674533145555
H	-3.27196442742453	1.13761927056274	-5.82404833678320
C	3.93095381162518	-0.21389894450896	-2.08040854666178
H	4.15269404201683	-0.15600280342054	-0.99754133121633
H	4.53105057174765	0.58304348076736	-2.55910235087437
C	3.36805045161825	-1.58193211884835	-2.63343637481443
H	3.76614185950004	-2.37879228345016	-2.15327799804145
H	4.13199866940717	-1.62813684790734	-3.71413066094796
C	5.86368372651090	-1.85744218162355	-2.41979002682043
H	6.12844958828740	-1.84847355523000	-1.34716484174855
H	6.14626264745926	-2.84267416348781	-2.82644417928189
H	6.48724976943573	-1.09888854445759	-2.92440435388336
H	3.47010570775599	-5.77440477030168	0.99040559552589
H	2.57850288558840	-5.77311505355041	2.52720505114629
H	4.13325029039258	-4.90864382323738	2.40255361301814
H	-4.15155114530151	-4.89288966689297	-2.40338525860608
H	-3.49237258105756	-5.76101492729470	-0.99091660046080
H	-2.60044699013456	-5.76393330849004	-2.52758236386359
H	-3.12460119089561	5.74989254383066	1.82968452326113
H	-1.86427345592609	5.74308105291242	3.08206109710647
H	-3.39970884008522	4.87961000837995	3.36220400775937
H	3.41677477349588	4.86416250459205	-3.36930255032791
H	3.14459317890509	5.73722060410546	-1.83783400790067
H	1.88419335048984	5.73301100635934	-3.09013889678847
H	3.89964976565706	-2.54344411641556	2.31913967779696
H	-3.90904297315377	-2.52896524884102	-2.32001459555636
H	-3.21566721163422	2.51682163184609	3.19743779130325
H	3.22511035392470	2.50214379823373	-3.20138271797460

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Bis-dbdmp triplet

Cu	0.04168667422233	0.05882339884879	0.02489498248287
N	-1.01225963604186	-1.46231586738035	0.75225841172660
N	1.23556346502449	-1.37542549074842	-0.66249818549418

N	-1.14616877487458	1.47132829209564	-0.71533762351939
N	1.08668334151249	1.59929520403672	0.72213026724086
C	-2.05748711666224	-1.44119251160070	1.61776631937921
C	-2.57853935798356	-2.63961273237600	2.14578454883089
C	-2.06316190085831	-3.90018743770743	1.80059928660471
C	-2.67727958034085	-5.16518026632904	2.34510017694626
C	-0.93212983686481	-3.92616140876656	0.93459233527473
C	-0.26284515708195	-5.12547525847488	0.51102420173702
H	-0.64261494502338	-6.09178668379654	0.85511219656628
C	0.83347626965395	-5.08507706798670	-0.32167378956397
H	1.30292790100725	-6.02034005813604	-0.63990539253477
C	1.38757673585908	-3.84003033703081	-0.77834364812289
C	2.51230507604904	-3.73125704409759	-1.64613825416989
C	3.24304045686666	-4.94719089337999	-2.15737445823021
C	2.90774213980649	-2.43759883806161	-2.02526056019959
C	2.27591974892392	-1.27962557699688	-1.52874713230986
C	0.75621047374477	-2.63663675282246	-0.33970474616723
C	-0.41615852120922	-2.68106766993606	0.46271589206968
C	-2.19698779606693	1.35261415510573	-1.56528175769763
C	-2.84215519245662	2.49611543486298	-2.07719536613624
C	-2.44059971363905	3.80011870248968	-1.73977540400410
C	-3.18116317233726	5.00134442108443	-2.27128423581461
C	-1.30738210681385	3.93161069842288	-0.88753665800717
C	-0.75466176583551	5.18957488987680	-0.46505929243447
H	-1.22632703853173	6.11503140530260	-0.80767641359925
C	0.34240017180063	5.25416114274043	0.36416874852998
H	0.72312306118448	6.22998891488648	0.67902599789014
C	1.01173795301960	4.06751055368117	0.82279693743490
C	2.15006723773497	4.06958252421186	1.67830308530864
C	2.77143560696773	5.35097603960608	2.17409910465674
C	2.67299218205735	2.82014726728543	2.05415776386193
C	2.14145878495577	1.60606172005470	1.57554811721588
C	0.49381835985902	2.80823977477911	0.39087899415556
C	-0.67198617533150	2.74059039265080	-0.42024877701538
C	-2.62206782115563	-0.02661086469714	-2.01083076108225
H	-2.43517134606629	-0.75815174200821	-1.20686027517445
H	-3.71009669705474	-0.02445995554267	-2.20546349834625
C	2.69466944461341	0.28652428499650	2.05937076237179
H	2.59044820836077	-0.47849993634925	1.27163713482516
H	3.77466495047391	0.40064403322769	2.26475537797255
C	2.73457660022096	0.09433040350582	-1.96454347445767
H	2.02421512975017	0.84311409295473	-1.57382453262988
H	2.67127116763223	0.14315966283146	-3.06976163464392
C	-2.64150568831870	-0.10483916745420	2.01907022292937
H	-2.00267294041261	0.69592562219442	1.60844742248826
H	-2.58379614599616	-0.02236537403317	3.12258313442255
C	1.98722233489060	-0.20602371727053	3.34848333031656
H	0.90741304372977	-0.33677617807101	3.13832349684502
C	2.05934489872003	0.57773979423543	4.12691771802145
H	2.57636910887579	-1.52350217516303	3.87999230788584
H	3.65662271956897	-1.38367816909512	4.07995558526710
H	2.50740924865177	-2.29810609012530	3.09144158152888
C	1.87613637885067	-2.01706800861469	5.15475607820884
H	0.80097170804033	-2.19971159039870	4.97680560473955
H	2.32129948012965	-2.96034724660050	5.51469544316510
H	1.95889991823037	-1.27619755418952	5.96993791735373
C	4.17520799522025	0.46151271944139	-1.53946709487203
H	4.25648767029030	0.41817678887977	-0.43681221218391
H	4.88110119667814	-0.29676560052642	-1.92974337076800
C	4.59611197636046	1.85558880930700	-2.03528095796961
H	4.49959750040610	1.89403757448864	-3.13808306390011
H	3.88973234846973	2.61062380167127	-1.63846122838415
C	6.03068991007088	2.22447128158079	-1.62991084011188
H	6.30482738020440	3.22763337672284	-1.99861131988526
H	6.14946748414089	2.22696474577897	-0.53131635120364
H	6.76141513980373	1.50604444751165	-2.04252040525745
C	-4.10936054342095	0.11774069228509	1.58690933708367
H	-4.18545878994356	0.03933430170759	0.48584081635577
H	-4.74313661755839	-0.69185125949581	1.99733141901515
C	-4.65641380612905	1.47962966457550	2.04784390410621

H	-4.56418814753463	1.55492135235721	3.14911105129497
H	-4.02199447873515	2.28577164334813	1.63043609328299
C	-6.11860422171984	1.70506149713225	1.63604464943350
H	-6.48380120048465	2.68782848421332	1.97988727012421
H	-6.23665092928136	1.66894552956429	0.53795987816543
H	-6.78046254645717	0.93324017475524	2.06798679093945
C	-1.88294127856332	-0.47741872212808	-3.29743224972864
H	-0.79313298500391	-0.49391368290956	-3.09943700053184
H	-2.04239583890143	0.27597519324374	-4.09271784906991
C	-2.34236619082580	-1.85975668469185	-3.79096456240692
H	-2.18541063139546	-2.60504712256612	-2.98695818806752
H	-3.43362838469905	-1.83450703537832	-3.97805201643004
C	-1.61154979762643	-2.30953064986527	-5.06480226174305
H	-0.52121299693555	-2.37776797864716	-4.89890157715665
H	-1.96276986360212	-3.30136039656194	-5.39709829780748
H	-1.77956855542653	-1.60029874003340	-5.89487059996490
H	4.07054823473744	-4.66016434804298	-2.82513150862094
H	2.57152556609707	-5.61877496171996	-2.72319781198866
H	3.67030813889528	-5.54158033047778	-1.32885747563494
H	-3.04469301285263	-5.81957106501826	1.53327599700489
H	-3.52973671222423	-4.93933290148464	3.00492900901123
H	-1.94687652598436	-5.75484793300754	2.92901107392645
H	-4.02156218522555	4.69562342016247	-2.91420877656578
H	-2.52020704344169	5.65445132365828	-2.87030208323910
H	-3.59148106702196	5.62116314817874	-1.45299061571034
H	3.11948501676612	5.98462514055155	1.33776940308396
H	3.63781884949314	5.14582733968504	2.82247420687678
H	2.05082944970643	5.95358497704064	2.75710907717680
H	3.74387236397096	-2.31132580153519	-2.72042581291424
H	-3.42332600131259	-2.57382382670082	2.83885251056142
H	3.53243442057664	2.77479439747132	2.73072775753400
H	-3.69348184361266	2.34925405475116	-2.74960932775926

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Bis-bfp reduced

Cu	-0.00010280873897	0.00004608944385	-0.00009110100917
N	-1.48426771516053	0.95743512277312	0.93328756593231
N	-1.48412655077236	-0.95783585066621	-0.93322892116406
N	1.48396086526975	0.94751783960639	-0.94399577329593
N	1.48438745349766	-0.94702293454947	0.94358528212949
C	-1.46636893445035	1.91984296792830	1.87173090630526
C	-2.63367257701483	2.48738123146927	2.42125506588895
H	-2.54788898833515	3.26617263279750	3.18087069988505
C	-3.87723669262011	2.04045228544213	1.98293436702045
H	-4.79892782902952	2.46454451187296	2.39355510451736
C	-3.94227474675019	1.02621787173294	0.99650314049784
C	-5.17496903420621	0.49244882228048	0.47848000899720
H	-6.11922522509504	0.89002750938065	0.86401092353054
C	-5.17489571544404	-0.49409491668824	-0.47770465977904
H	-6.11909272611917	-0.89199375782788	-0.86305023602709
C	-3.94212208259057	-1.02744420032471	-0.99597107871757
C	-3.87693284295090	-2.04164834857339	-1.98242326276215
H	-4.79856044300773	-2.46604758648160	-2.39286953705522
C	-2.63330315150170	-2.48815446023292	-2.42098868492370
H	-2.54740443724092	-3.26690979024685	-3.18062825069739
C	-1.46608439894435	-1.92023087320730	-1.87168171133403
C	-2.70533654925632	-0.51722099335108	-0.50197053996892
C	-2.70541353827630	0.51640947013546	0.50226473685288
C	1.46577968839817	1.89895484299082	-1.89356323594720
C	2.63291620315465	2.46047109648844	-2.44957443132418
H	2.54691217412255	3.23043355264739	-3.21811221320278
C	3.87660875530013	2.01905670590499	-2.00605685669903
H	4.79817625205450	2.43876106585661	-2.42143659167955
C	3.94194194637011	1.01613737041526	-1.00815271804822
C	5.17479587768289	0.48865027467598	-0.48410631192719
H	6.11893342883623	0.88213718597490	-0.87410004543776
C	5.17501544839759	-0.48699740988026	0.48318971150383
H	6.11932999640591	-0.88018611464350	0.87305556536053
C	3.94239900015519	-1.01487339135235	1.00740305939944
C	3.87751689263947	-2.01781484582245	2.00531422591964

H	4.79927290573681	-2.43722997872928	2.42056789693416
C	2.63402373712552	-2.45962073759244	2.44900104103271
H	2.54836690835134	-3.22961181510047	3.21754890388463
C	1.46663499290909	-1.89846721791705	1.89315203468959
C	2.70545253700280	-0.51071439336624	0.50759308082491
C	2.70522286433840	0.51158939089771	-0.50817323290113
C	0.08794550617956	2.35494356034686	-2.35619118796929
C	-0.08830266740725	-2.38252931607624	-2.32817464129074
C	-0.08865465870037	2.38260534917237	2.32795608772547
C	0.08900730907795	-2.35488753427615	2.35597004862729
F	0.18506795191349	3.29920363366953	-3.32144538805162
F	-0.63061773989198	1.31585912993119	-2.85900960383546
F	-0.62815776829233	2.88180598980850	-1.32742912981115
F	0.63305096957353	1.34968162202371	2.83881525933341
F	0.62441967959523	2.90165099277367	1.29309122861688
F	-0.18601221352893	3.33536585148196	3.28479815599948
F	-0.62981535298430	-1.31602594906644	2.85888041209123
F	-0.62706990088664	-2.88198090021559	1.32730825929245
F	0.18655658114960	-3.29911084398509	3.32121608524974
F	0.62515433337617	-2.90131592983351	-1.29344309940516
F	-0.18552652544676	-3.3533976519697	-3.28498153884442
F	0.63294777602954	-1.34936878071926	-2.83919369093353

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Bis-bfp oxidized

Cu	-0.00001193044216	-0.00000312568264	0.00062334819029
N	-1.49939239768581	-1.10809423661215	0.75491793263859
N	-1.49805893895633	1.10967791678584	-0.75471950457461
N	1.49944140458460	1.10814744711249	0.75478126038457
N	1.49798652607303	-1.10967869675562	-0.75475853451384
C	-1.45490732636590	-2.12650379926756	1.62698547035437
C	-2.62387156287484	-2.73393815713291	2.13507594996642
H	-2.53506671563427	-3.56079963960383	2.84312333652897
C	-3.86902271267535	-2.26354658812953	1.72739173965201
H	-4.78550924014592	-2.73658898543573	2.09426582726234
C	-3.94724678296081	-1.14546120513723	0.85638216431936
C	-5.17997944038316	-0.54494286207815	0.41595921179673
H	-6.12502743865557	-0.97951840313672	0.75576734235636
C	-5.17931691764669	0.54966316100931	-0.41742857735879
H	-6.12383676420935	0.98504460534724	-0.75767415033522
C	-3.94587262804442	1.14914217434142	-0.85728129316522
C	-3.86632319377852	2.26717799250676	-1.72823103773103
H	-4.78224562670174	2.74101258857577	-2.09549117873775
C	-2.62059065581133	2.73648284439187	-2.13536865508863
H	-2.53075428711684	3.56327559142930	-2.84336462728529
C	-1.45235799168853	2.12801951641033	-1.62680087934638
C	-2.71326850984823	0.58941468664535	-0.41321163784405
C	-2.71397628645621	-0.58676029789424	0.41286583503949
C	1.45502040332778	2.12663132646611	1.62675923817186
C	2.62402492869601	2.73412018226743	2.13470079805093
H	2.53527153268610	3.56105128928830	2.84267228934211
C	3.86914601941773	2.26368540096181	1.72697815360227
H	4.78565891404567	2.73676133636670	2.09374311658468
C	3.94730394386194	1.14551005350937	0.85607674877239
C	5.18000072497529	0.54490799857640	0.41566843147616
H	6.12507599443122	0.97949681320552	0.75538405289941
C	5.17927500023170	-0.54980606655459	-0.41757714086711
H	6.12377147362316	-0.98526041094630	-0.75779430977249
C	3.94579740020665	-1.14929298448986	-0.85732586422343
C	3.86618455008468	-2.26742978465328	-1.72813915743461
H	4.78207998924129	-2.74135435912694	-2.09535022084794
C	2.62042472896283	-2.73671894348298	-2.13520931218156
H	2.53054187998417	-3.56359309598503	-2.84310423673940
C	1.45222785389079	-2.12812657779460	-1.62671335364188
C	2.71322798858586	-0.58945403651727	-0.41330162814198
C	2.71400112607721	0.58678705607631	0.41268225658468
C	0.07457686741640	2.59167223413529	2.09177580397577
C	-0.07131547437302	-2.59177511580968	-2.09134083343828
C	-0.07442113283312	-2.59151656176948	2.09189583328221
C	0.07116775086821	-2.59187279774761	-2.09121525284956

F	0.15083293177928	3.15080393873601	3.30995209067218
F	-0.47948380806629	3.48152792469236	1.23893511616432
F	-0.77144704309111	1.51413511071904	2.16356573771876
F	0.47948982035757	-3.48153541320440	1.23912174358055
F	0.77165040105026	-1.51399262426574	2.16338009411617
F	-0.15052184499610	-3.15044360431409	3.31017023933266
F	-0.48359857793806	-3.48090337540589	-1.23796146587530
F	-0.77374100286508	-1.51350558561543	-2.16314045592675
F	0.14653967057584	-3.15148428344520	-3.30923701490697
F	0.77359183945743	1.51339627771757	-2.16323638793217
F	-0.14670137037073	3.15134455400827	-3.30937623749797
F	0.48346493812282	3.48082736509315	-1.23812121455840

#=====END

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Bis-bfp triplet

Cu	0.00000480362454	-0.00025162216578	-0.00008962719822
N	1.47051397136906	1.11986319750756	0.73021561285789
N	1.47043556283156	-1.12030823939792	-0.73038741613845
N	-1.47044308301331	-1.12028036991697	0.73033561930126
N	-1.47049668328705	1.11996208822050	-0.73014937396545
C	1.43453237527248	2.12695625940012	1.63127986455649
C	2.59581390776058	2.71466223512561	2.15413063762071
H	2.50463161365440	3.52993728531756	2.87385173082229
C	3.85310366822678	2.24718787415487	1.74438535491808
H	4.76824490833403	2.71580585668719	2.11865917214007
C	3.92874875305336	1.14254173939701	0.86918688687564
C	5.16017110872384	0.54152316262468	0.42265717866204
H	6.10518509517248	0.97323758187229	0.76754806876425
C	5.16013663490695	-0.54223132216052	-0.42267474309306
H	6.10512509056419	-0.97398069168974	-0.76759259488553
C	3.92868126362804	-1.14312725643758	-0.86929170570670
C	3.85299358063424	-2.24758808897462	-1.74471976884346
H	4.76811373702777	-2.71617061785744	-2.11908712520003
C	2.59568093181653	-2.71473894191437	-2.15477337163343
H	2.50447099714132	-3.52970064308604	-2.87484627912718
C	1.43441855253013	-2.12705750273645	-1.63187705007636
C	2.69851557045531	-0.58229301129403	-0.40874104451277
C	2.69855196316183	0.58169165718281	0.40872537695942
C	-1.43443926747294	-2.12710103917191	1.63173484213481
C	-2.59571411171722	-2.71483838761836	2.15455401845331
H	-2.50451781402928	-3.52986096385227	2.87455974445595
C	-3.85301720197167	-2.24765898764300	1.74451512511020
H	-4.76814188255718	-2.71628198696182	2.11882170491336
C	-3.92869422388601	-1.14312138920361	0.86918283519338
C	-5.16014097945610	-0.54218869337000	0.42259751616183
H	-6.10513546784624	-0.97396694254835	0.76746231569782
C	-5.16015834202286	0.54164115269501	-0.42263851571887
H	-6.10516528966240	0.97339118779284	-0.76750385030585
C	-3.92872705917913	1.14268947854770	-0.86910553096864
C	-3.85306959166314	2.24740642049167	-1.74421872773392
H	-4.76820754788451	2.71606195677391	-2.11845294742511
C	-2.59577416312158	2.71489303965565	-2.15393352500904
H	-2.50458016015791	3.53022031741683	-2.87359463127796
C	-1.43450024374778	2.12712147613059	-1.63114301412279
C	-2.69854168902288	0.58179219102632	-0.40868198585689
C	-2.69851656734268	-0.58224746954300	0.40870879335825
C	-0.06191803676601	-2.59616144154070	2.09854995036934
C	0.06188409579498	-2.59606522439115	-2.09868617953258
C	0.06198237830449	2.59663528464153	2.09736039806701
C	-0.06194510681754	2.59679984846918	-2.09720298703253
F	-0.15339945336139	-3.24179727514398	3.28276197214061
F	0.53605475702932	-3.43219446867535	1.21511823224988
F	0.77250059778970	-1.52548861751344	2.26810778526076
F	-0.53535850726537	3.43240341002553	1.21324102533577
F	-0.77282627400223	1.52629898084645	2.26709532982196
F	0.15318900790546	3.24283117451032	3.28128712282236
F	0.53538288679928	3.43258365712791	-1.21309530057921
F	0.77287148577138	1.52645562691556	-2.26690401091209
F	-0.15313441999155	3.24296759213415	-3.28114626566534
F	-0.77247587350611	-1.52533602402060	-2.26826466409144

F 0.15331974968215 -3.24173302811754 -3.28287894217239
F -0.53614800821412 -3.43203048574482 -1.21523103623944

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Bis-dbtmp reduced

Cu 0.00302404887794 -0.00072043959520 0.00496210695912
N -1.50521325269947 0.59997724440524 -1.19663127475391
N -1.51949882997579 -0.56469869310800 1.20663092046167
N 1.50239344699289 -1.22165197004858 -0.57879161616602
N 1.53443217583330 1.18148382127458 0.58601109121621
C -1.44351246586936 1.19728172464533 -2.40679081446708
C -2.61796191246295 1.60778110487593 -3.11339580605924
C -2.50227039902981 2.32371047602192 -4.44587619705305
C -3.88411419702101 1.34348361899721 -2.55624577342954
C -5.16693011749908 1.72411576752902 -3.25935942081300
C -3.95140737461583 0.69236089958463 -1.28478630841062
C -5.18054725052114 0.36899930857610 -0.61135549805169
H -6.13183762521064 0.62233230252321 -1.08690333236273
C -5.18818939723131 -0.25049366976175 0.61772228598970
H -6.14546597222667 -0.48268587752432 1.09204834575973
C -3.96735490194888 -0.60150223671149 1.29242226425838
C -3.91599857624553 -1.25449075930094 2.56372802145770
C -5.20765291611532 -1.60563830283051 3.26601561543670
C -2.65667269275331 -1.54851494376758 3.12142927145518
C -2.55850837713855 -2.26882645134837 4.45295453459743
C -1.47252197561976 -1.16401684141102 2.41639728601316
C -2.73919651390338 -0.28823061517094 0.65109067527970
C -2.73133090205389 0.35139435554880 -0.64219864169006
C 1.43192726967960 -2.43097280599586 -1.17681411409252
C 2.60170999574566 -3.15162855463054 -1.57611413318039
C 2.47688339538464 -4.48244289458736 -2.29361431081734
C 3.87185871090696 -2.60995795883863 -1.29913358340466
C 5.14973505671725 -3.32867225063728 -1.66706208249419
C 3.94814266281636 -1.33942259607289 -0.64718681890313
C 5.18213065339346 -0.68088121925538 -0.31184655130045
H 6.13000999187595 -1.16795061312534 -0.55590757669014
C 5.19859847403289 0.54814456714898 0.30757447930813
H 6.15921165037115 1.01098999361594 0.54895462226893
C 3.98264080387453 1.23761565719013 0.64661323854818
C 3.94036440173376 2.50973391761663 1.29868889109465
C 5.23699799309553 3.19661667321475 1.66175694846491
C 2.68511751889188 3.08275164018703 1.58034705885475
C 2.59591350343057 4.41567796398063 2.29920992168546
C 1.49630499422452 2.39188538151577 1.18463509991888
C 2.74992924272560 0.61110075503128 0.32147707523552
C 2.732644498529353 -0.68207035139067 -0.31817862203497
C 0.02942224774106 -2.97238419607882 -1.35544232134796
H -0.65780952332860 -2.12118780926260 -1.20315190498973
H -0.12526370868924 -3.33441632749827 -2.38940531353328
C 0.10841501541334 2.96819561735360 1.36828280763792
H -0.60043604129190 2.13477256371435 1.21650541397085
H -0.03409419504377 3.33208856424363 2.40336646637470
C -0.07962160378255 -1.36056159538505 2.97611626180824
H 0.62060383468577 -1.21560618112245 2.13423824631793
H 0.05764839971822 -2.39678025530495 3.33874555099307
C -0.04592180495255 1.36296683510469 -2.96477708919582
H 0.6499439077949 1.20461358326590 -2.12171952805276
C 0.11374514583440 2.39543271648325 -3.32892156154120
H -0.23284487386824 4.10149981128249 0.37096366034711
H -0.12834172536414 3.71002060934731 -0.65927145581089
H 0.50137943438544 4.92435353321902 0.46370330191825
C -1.65303956900659 4.65627197337477 0.57456326845164
H -1.75215435777340 5.03127439464862 1.61224124799494
H -2.38303973064440 3.82916308188149 0.47683338059945
C -2.00413186798032 5.77871151838455 -0.41307312137937
H -1.94567581962387 5.42569298814544 -1.45855023843491
H -3.02698100261070 6.15659319276609 -0.24328964591391
H -1.31165768541470 6.63350324384553 -0.31146349401811
C 0.28413728375930 -0.36606000821011 4.10487276397259
H 0.18365835341818 0.66496712760394 3.71441501457170

H	-0.44078659331620	-0.45237888891270	4.93662739531778
C	1.70917841994502	-0.58178051231463	4.64233863153193
H	1.80404305290274	-1.62031193939587	5.01607438786986
H	2.42988256344229	-0.49009894187481	3.80643100145362
C	2.08218057268238	0.40270825805716	5.76047309092756
H	3.10814663972754	0.22441183382495	6.12577523969193
H	2.02803510352988	1.44869240715125	5.40826726280616
H	1.39941966210261	0.30668274192394	6.62368039459608
C	0.29842199999724	0.35898112087662	-4.09126726705694
H	0.17806646018826	-0.66897031514078	-3.69834585767087
H	-0.42469960657337	0.45736962490195	-4.92326265413895
C	1.72740591466633	0.54570649335408	-4.62912517967904
H	1.84236255158206	1.58122426923732	-5.00557739360730
H	2.44618329175193	0.44231688674870	-3.79291931528037
C	2.08140280680913	-0.44874113635344	-5.74461660144613
H	3.11062037830704	-0.29119753900211	-6.11031373199356
H	2.00712699726260	-1.49254245674936	-5.38961539774113
H	1.40063305645254	-0.34188714151831	-6.60812523817859
C	-0.33697793051419	-4.09498497747441	-0.35494739094478
H	-0.22028476634998	-3.70400948510056	0.67417493251673
H	0.37676619644780	-4.93565733969035	-0.44786090809371
C	-1.77080501136786	-4.61533474327381	-0.55372516615001
H	-2.48019644764706	-3.77055271329113	-0.45532610810290
H	-1.88193283187254	-4.98948100441581	-1.59049517769044
C	-2.14625405847853	-5.72732986899022	0.43676167018813
H	-2.07589962004590	-5.37425399604219	1.48148774275241
H	-3.17857528536493	-6.08030146606532	0.27072211218804
H	-1.47523926512003	-6.59897852325857	0.33439853645044
H	-2.90022953757981	1.70972391865819	-5.27443913651492
H	-1.46224944747945	2.57316161424892	-4.69665261306339
H	-3.07213129636624	3.26926194379216	-4.44219700471169
H	-4.99147311213882	2.15332874525382	-4.25487420976402
H	-5.73940054193100	2.46571601781213	-2.67193717159682
H	-5.82225692308699	0.84413035964369	-3.38995261729603
H	-5.84588142294939	-0.71221491810003	3.38938597577133
H	-5.04306932480693	-2.03178894441150	4.26469334640303
H	-5.79318231471682	-2.33957114479219	2.68175410633225
H	-1.52512657924064	-2.54600644103202	4.70215523452936
H	-3.15311940173770	-3.19896576175953	4.44878782703840
H	-2.93920645460070	-1.64559255841435	5.28275491715900
H	2.85640544987032	-5.31626128497297	-1.67506332957956
H	3.05796273526339	-4.48633584426037	-3.23228807308277
H	1.43666115649105	-4.71934519588948	-2.55552717601514
H	4.96647148516874	-4.32277100860891	-2.09629828992098
H	5.79546844523270	-3.46553310938961	-0.78097789155395
H	5.73576804549849	-2.74922308585112	-2.40434149771218
H	5.88427662710183	3.31335342249868	0.77395090644452
H	5.80937010108951	2.60499285194613	2.40013287622653
H	5.08030669757415	4.19677876224420	2.08741370239214
H	1.56310736994058	4.67631157629635	2.56793345527490
H	2.99066606995845	5.24093283797741	1.67867519421913
H	3.18293691218200	4.40543464972594	3.23408788967512

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Bis-dbtmp oxidized

Cu	0.00249607547551	-0.00847411327291	-0.00100477474228
N	-1.18458443360708	-1.49788821176514	-0.63430456212750
N	1.17787416277598	-1.50986630666280	0.62708998470676
N	0.96779036045295	1.48921994007782	-0.93298907086752
N	-0.95159891815275	1.49277833602700	0.93843546685905
C	-2.32503382177179	-1.41883809311503	-1.35511712943725
C	-3.02470196116226	-2.59944838129041	-1.77298486128543
C	-4.31316854140409	-2.49230007113513	-2.56423390307955
C	-2.51198469114042	-3.86475924299912	-1.42638711236229
C	-3.21649129622094	-5.14432182397504	-1.80227651059654
C	-1.27120260073621	-3.93566340828823	-0.71246277491898
C	-0.62085815262524	-5.16406488456070	-0.34815416814185
H	-1.08820697255758	-6.11496929036447	-0.61496935443661
C	0.57757882481214	-5.17244325715413	0.32927188735846
H	1.02001577433128	-6.13204296121718	0.60543104616838

C	1.25043588369262	-3.95363653523624	0.69030309628790
C	2.49647658544358	-3.88894601241021	1.39571046159959
C	3.24522859070870	-5.14301340107018	1.76975954592919
C	3.00268673570640	-2.62626756816867	1.76565632446844
C	4.28301645553988	-2.54377336864669	2.56959818087803
C	2.31548301490707	-1.43993944782617	1.35370376097361
C	0.62531893512755	-2.72789052689908	0.33675677961771
C	-0.63847566009279	-2.72040313964264	-0.34933654516599
C	1.83384532282628	1.41252251995518	-1.96805000549623
C	2.31250900363201	2.59434160197526	-2.62383483722356
C	3.21727570769440	2.49013163767020	-3.83453692984044
C	1.93696964428583	3.85938591713082	-2.13062461292831
C	2.48071544441625	5.13318930302563	-2.72807673008494
C	0.99375510789232	3.92847735850105	-1.05358143726173
C	0.47727050376005	5.15383071176341	-0.50694563713290
H	0.82447131990523	6.10764647894711	-0.91106752080038
C	-0.44909387869146	5.15526570450828	0.51222823323990
H	-0.79581788196025	6.10997248132760	0.91474571357790
C	-0.96757636946479	3.93146821950009	1.06009011115344
C	-1.90949926737191	3.86620538776266	2.13849267783206
C	-2.44395988287127	5.14463707082459	2.73435551869553
C	-2.29158760721962	2.60271765483999	2.63040379633502
C	-3.19699278623853	2.50053465649762	3.84097691843648
C	-1.81803850367885	1.41920320882607	1.97329409667361
C	-0.49163879611722	2.71096038301156	0.51707280504629
C	0.51294059219250	2.70924839850334	-0.51116249016335
C	2.26426797210798	0.02423820208572	-2.38715447190507
H	1.59110226898230	-0.70182874520541	-1.89867755372730
H	2.10474975483649	-0.09354297074638	-3.47573533212939
C	-2.25356804499413	0.03230835479277	2.39183303160442
H	-1.58342077400910	-0.69600431508717	1.90251619420912
H	-2.09356172999666	-0.08651195509862	3.48024352992284
C	2.78455519807376	-0.05852735080126	1.74802111821256
H	2.35269934379888	0.67444568544061	1.04561757434398
H	3.88168588963329	0.01861786491880	1.65003584894335
C	-2.77939632507923	-0.03071204340377	-1.74423397553792
H	-2.30258878635874	0.69679295943773	-1.06582977912668
H	-3.86960326940752	0.07554053018132	-1.60359604268391
C	-3.72363203469782	-0.31998865687441	2.05454111587243
H	-3.86911224815298	-0.25634126704071	0.95945295466710
H	-4.40392372013582	0.43060857417328	2.49673943412103
C	-4.11501349308173	-1.72211644898593	2.55382273541711
H	-3.94983848217034	-1.77768573051247	3.64726995116263
H	-3.43576743241263	-2.47272434764244	2.10321767279257
C	-5.57421769527247	-2.08030303424115	2.23647175268941
H	-5.76857617806779	-2.06025132200599	1.14883621421345
H	-5.82397800620015	-3.08971320769933	2.60368596286489
H	-6.27417729416681	-1.37156319904830	2.71259297487507
C	2.36724265981183	0.32523227799143	3.19397894994798
H	1.26163989283195	0.31451350278532	3.26178611549732
H	2.72331989996139	-0.44256355309158	3.90611582156024
C	2.90636425591334	1.70455362616870	3.61267483603783
H	4.01099499423285	1.69999156112421	3.53901670016881
H	2.55464314692589	2.46954632337535	2.89258482658564
C	2.48765706322121	2.09659218847160	5.03740752160983
H	2.89014198521570	3.08660483756739	5.30950774139595
H	1.38814940539988	2.14116760854440	5.13777711290913
H	2.86193896100544	1.37041748173266	5.78006937306588
C	-2.41010295540738	0.33139322032652	-3.20841367361758
H	-1.30953088963111	0.28048660947469	-3.32280746690745
H	-2.82418665189379	-0.42529756848490	-3.90047769224192
C	-2.91607824552711	1.72792298108663	-3.61129401129358
H	-4.01565419188340	1.76532753626857	-3.48784934436864
H	-2.50336688898077	2.48250578347365	-2.91281129417757
C	-2.54782631823370	2.09702888570052	-5.05597138143580
H	-2.92403195682394	3.10058482176512	-5.31584959443810
H	-1.45316604903732	2.09857319194224	-5.20646869505731
H	-2.98315417110711	1.38245421441859	-5.77624683599332
C	3.73280414197417	-0.33327907438693	-2.04883112055033
H	3.87968107940176	-0.26408092671413	-0.95423626624148

H	4.41615519386462	0.41157555108418	-2.49597015735616
C	4.11716654859863	-1.74007523771292	-2.54032575286145
H	3.43496520085210	-2.48488344183130	-2.08459156279654
H	3.95081338928290	-1.80146387733643	-3.63326205047672
C	5.57501728455010	-2.10296943239736	-2.22213167967500
H	5.77066094581642	-2.07598821261500	-1.13478159199960
H	5.81969648433902	-3.11608062960832	-2.58249245466076
H	6.27785350846416	-1.40079529425692	-2.70368317002813
H	4.49768618315219	-1.53107627883373	2.93429583825431
H	5.15202737773868	-2.86716892857221	1.96644247919999
H	4.24153051692523	-3.20844448187001	3.44943688778035
H	2.98901658793705	-5.99729900554227	1.12728454525462
H	3.02420977896462	-5.43442741515691	2.81489007623843
H	4.33475451683428	-4.99542171207236	1.70501998663489
H	-4.19111142794645	-4.97058465316982	-2.27555670159363
H	-3.38354638429827	-5.77933403673718	-0.91418361232773
H	-2.60442149336183	-5.73516656463678	-2.50896297478288
H	-4.22843452675686	-3.00947822818944	-3.53598530220586
H	-4.60178854182667	-1.45437529332121	-2.77329662630121
H	-5.15246085915527	-2.96087815522986	-2.02027432425126
H	-3.24314867354165	1.48199718650780	4.24941493705629
H	-4.23246379059498	2.80488822961201	3.60182642708815
H	-2.84459622337301	3.16033567472657	4.65139375719410
H	-2.76288276641855	5.84709955745697	1.94569187395791
H	-1.66559051007044	5.65908168801036	3.32947410912086
H	-3.30581713193322	4.97446911798694	3.39294930349963
H	3.37312625246274	4.95967054219754	-3.34422849724552
H	2.75588780423574	5.85701465302394	-1.94299650061816
H	1.72363717431111	5.62342406719147	-3.36968776652561
H	2.87457726493437	3.16158947147149	-4.63942784910545
H	3.24995623732492	1.47437202149778	-4.25134230270514
H	4.25670311759630	2.77848987417098	-3.59224898476365

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Bis-dbtmp triplet

Cu	0.03801188602794	0.03613347172513	0.02435359558498
N	-0.98097355255629	-1.48476341191479	0.81333745762373
N	1.19216630179295	-1.40661996781110	-0.72487207127129
N	-1.13327724728900	1.45418823277796	-0.74290601806281
N	1.06804784338134	1.58020423853052	0.75085129284571
C	-1.97284474135723	-1.44171253220627	1.74350597512136
C	-2.47126638379980	-2.62514317472366	2.34800165567990
C	-3.54303721667179	-2.56370825304393	3.41625142224613
C	-1.97546726514713	-3.89237953729961	1.93457595718705
C	-2.57373915423547	-5.15325992102072	2.51153682418210
C	-0.90019182395348	-3.93369658249797	1.00438825669938
C	-0.24914922815676	-5.13226645441424	0.54197546218719
H	-0.59358350673514	-6.10317743676814	0.90668263203972
C	0.79914575463678	-5.09674643354611	-0.34765670477060
H	1.23191324799473	-6.04182192961245	-0.68508219084986
C	1.33756535025041	-3.85706056154674	-0.84522705562069
C	2.40562426566653	-3.74373286672341	-1.77780866473398
C	3.11903047083519	-4.96053701130118	-2.31734846418881
C	2.78198123347080	-2.44872011434880	-2.22937911956245
C	3.84336126452590	-2.31946537042798	-3.30197508838529
C	2.17653322360748	-1.29933520833606	-1.65778988479861
C	0.72613088144379	-2.65787822299595	-0.37239071503953
C	-0.40116623512065	-2.69738405845182	0.49636089452029
C	-2.15046263140728	1.31987856467490	-1.63447335377461
C	-2.80663679486073	2.45183679312560	-2.18511891695728
C	-3.93917679783148	2.29377342256886	-3.17890980554259
C	-2.42192583461341	3.75811859544193	-1.77649908507766
C	-3.17740898676420	4.95657178001385	-2.29897671528095
C	-1.30823868975617	3.89940804196368	-0.90258996350601
C	-0.75672852242967	5.15409868825135	-0.46044789070459
H	-1.20804501026393	6.08802821728869	-0.80438238950443
C	0.32759504164743	5.21764859283830	0.38270638292092
H	0.68413510358819	6.19952309786204	0.70359486478466
C	1.00035659745190	4.03440659278550	0.85324728980007
C	2.12224959867422	4.02433129944269	1.72789556148836

C	2.75424804392856	5.30247580624258	2.22449843617801
C	2.63666738447652	2.77221556575120	2.16288908235774
C	3.78265706057621	2.75186118853034	3.15352338236847
C	2.09490020404328	1.56825138706711	1.64157005254402
C	0.48233965726397	2.78194568487711	0.40744676881395
C	-0.66926335406955	2.71526607302737	-0.42832716606163
C	-2.50315369122356	-0.09741857642705	-2.03509296770187
H	-2.20149274145894	-0.77942899696522	-1.22278460859768
H	-3.59619468599296	-0.20719667336612	-2.14819196697263
C	2.58790501546426	0.20276592273330	2.07319843613387
H	2.34378942453748	-0.52645738344487	1.28293960511912
H	3.68794226377525	0.20238294454732	2.17198469399828
C	2.58158360998281	0.10934411920827	-2.04295951379367
H	1.80934605714961	0.79833495562807	-1.65873215407270
H	2.56200640013809	0.20662326240681	-3.14558131697732
C	-2.50660172906467	-0.06592599190253	2.08848238749627
H	-1.79892638108510	0.68001601358773	1.68671905882133
H	-2.50074546207420	0.06305537616358	3.18800262678036
C	1.95135691728415	-0.27241265261637	3.40448089054443
H	0.85145618579757	-0.30850610267389	3.28007061248624
H	2.14548004426398	0.47112101335528	4.20113690809789
C	2.46931191235182	-1.65195816807853	3.84581113754039
H	3.57076125741720	-1.60917838362553	3.95522160442541
H	2.26879171447002	-2.38903306244078	3.04398166411074
C	1.83988689880442	-2.13275592962738	5.16162850128252
H	0.74192967418067	-2.21880349207898	5.07244620525681
H	2.23130426486222	-3.12232892664933	5.45346057156228
H	2.05373828597763	-1.43189891301491	5.98837562495612
C	3.96593335876257	0.56236175540142	-1.52304750391084
H	3.97661695092157	0.50103005563827	-0.41876772197117
H	4.74850332548068	-0.13445109743374	-1.87711093787110
C	4.31649225133828	1.99373984148694	-1.96472588303377
H	4.28337596675760	2.05227635083899	-3.07051072447939
H	3.53680248091415	2.68906659914681	-1.59721580285437
C	5.69569294120121	2.45104176873228	-1.46768227727203
H	5.91870794611871	3.48074057816924	-1.79571281725820
H	5.75102887139193	2.43082999426447	-0.36412335555087
H	6.49842038328948	1.79686684002646	-1.85254595252416
C	-3.92457392609499	0.24352081235617	1.55389757905616
H	-3.92545101224591	0.15035293674982	0.45179913605320
H	-4.64130023041044	-0.51199403607482	1.92655381740424
C	-4.40623666408078	1.64847383974655	1.95468994037584
H	-4.38210167736812	1.74084739748255	3.05841066174044
H	-3.69230731556666	2.40167422041546	1.56817589301578
C	-5.82003971744066	1.96354829167164	1.44447975024840
H	-6.13776800973967	2.97680604470303	1.74445034041494
H	-5.87000238471313	1.90877196271962	0.34183528981345
H	-6.56043957015813	1.24891084650892	1.84641999936887
C	-1.80208529197134	-0.54008280245908	-3.34501171085767
H	-0.70603126603047	-0.47079566007301	-3.20200630721501
H	-2.04993368064771	0.16538080278201	-4.16121086762571
C	-2.18162649591530	-1.97069573334233	-3.76382650455796
H	-1.93585691177157	-2.66869106490986	-2.93993286759824
H	-3.27922868501286	-2.03094419981708	-3.90019187908177
C	-1.47720072348014	-2.42110186327755	-5.05209595266300
H	-0.37874491151189	-2.40484754904744	-4.93366005522075
H	-1.76972782008044	-3.44832324065489	-5.32935112405815
H	-1.73147605220310	-1.76086505306359	-5.90055615380223
H	3.67222970627061	-3.04477309943073	-4.11616058937960
H	4.85743574097656	-2.52044326294450	-2.90620820707328
H	3.86473500302110	-1.31790813183062	-3.75527458120448
H	4.20563292639720	-4.78621095143621	-2.39143559399673
H	2.76818276748591	-5.21614265952049	-3.33622813220262
H	2.97272391858760	-5.85016812984025	-1.68787343799272
H	-2.34073410128394	-6.04522453611096	1.91224140514207
H	-3.67238566057659	-5.08018481499546	2.57722639889290
H	-2.20594164545551	-5.34121816817551	3.53910306707668
H	-3.66103026747502	-1.55497345330392	3.83760467704819
H	-3.30595262156988	-3.24335025819490	4.25303983690297
H	-4.53220380557899	-2.87267646971178	3.02715523699186

H	-3.80794449424089	2.97051437582259	-4.04126808507479
H	-4.91692677426420	2.54592852355218	-2.72491254127130
H	-4.01813182780151	1.27271283152432	-3.57636933253732
H	-4.26552861155174	4.77519701952994	-2.29529497969692
H	-2.89803132178476	5.18341908640444	-3.34628263970606
H	-2.99524925325401	5.86440439133673	-1.70618874017733
H	2.46810963778557	6.17903312981060	1.62596397651302
H	3.85543201037452	5.23699584188374	2.20486123794150
H	2.46902237023223	5.51070883209546	3.27403101756019
H	3.98147271894238	1.74946744724400	3.55628563906036
H	3.57633171506821	3.41415607453641	4.01266824659675
H	4.72267706613950	3.11388110255306	2.69442012852551

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Bis-tpg reduced

Cu	1.25746092302835	3.36096117978029	5.15996435037383
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C	2.36872208591472	6.14740112762225	4.51754042521405
C	2.68620818919811	7.17117230272011	3.59239087036683
C	2.61827744385992	6.97065018650627	2.21263899002834
C	2.23367089732897	5.66460230499482	1.75983255758714
C	1.89241741639133	4.69075819884855	2.74829585395438
C	1.44893304563799	3.37314165457906	2.33885545239171
C	1.47896990142153	3.01177628217860	0.95676390670587
C	1.07778696767168	1.67990640697051	0.60525902626076
C	0.63122597875230	0.85622522828706	1.63971906202822
C	0.59235019188666	1.29335088533704	2.98643257624800
C	2.21555428251660	5.27702929151874	0.37831821988193
C	1.86335819363438	4.00454498119678	-0.00543565721732
C	2.49835325499493	6.42101264785613	5.97174026779228
C	2.13239384497878	7.68495078656569	6.48890450045015
C	2.30274312905029	7.97712573792689	7.84872400355667
C	2.85255803636615	7.01679203248076	8.71299939984021
C	3.22121773897004	5.75869400598108	8.20951445994869
C	3.03760674182937	5.45930958100498	6.85336251129667
C	0.06337336823693	0.37608830676203	4.02837387660533
C	0.32911219622171	-1.01080940334278	3.95463868500813
C	-0.21640334947072	-1.89431752020361	4.89531512648388
C	-1.04730152743503	-1.41051458578440	5.91864782781460
C	-1.31777051826183	-0.03509227310122	6.00169164273775
C	-0.76054143606592	0.85126339138604	5.07112475458333
N	2.00130417932741	2.09774883688695	6.53464331553310
N	0.02451196573680	3.91760323578225	6.65587378096106
C	2.95860562199545	1.14375605823048	6.42361871394202
C	3.27087082970150	0.28856063475341	7.50894355002978
C	2.62517619818468	0.38690679853510	8.74162945116309
C	1.63283640872325	1.41339812598885	8.87889708661564
C	1.33936513457013	2.21619092917912	7.73323449642435
C	0.30352848271975	3.22787969916847	7.81135467016546
C	-0.36477242703588	3.46446261993862	9.05260752872103
C	-1.37606528225487	4.48090690743077	9.08580532810357
C	-1.59806617982443	5.19670339424643	7.90864043848534
C	-0.90266296038684	4.90481697535170	6.70907047998409
C	0.98189956554221	1.71950797973302	10.12018115887708
C	0.03382186869961	2.71079756109353	10.20616773291374
C	-1.25245990043028	5.66188257329385	5.47922178937177
C	-1.57376592827363	7.03643711178589	5.56701575206092
C	-1.97141230950748	7.75328975314468	4.43110600746526
C	-2.06958542025138	7.10688566551283	3.18843365007728
C	-1.75160217964640	5.74291215372257	3.08863846172482
C	-1.33725509282785	5.02915750824091	4.22069910313842
C	3.71801966028872	0.99525311816479	5.15469511129930
C	4.13191397212889	-0.28764322549874	4.72529108501419
C	4.90816634561812	-0.44070722334880	3.56940402202382
C	5.29688645935492	0.68555373487256	2.82627388646917
C	4.88797939781437	1.96366376321943	3.23925693013024
C	4.09775436433032	2.11628481632461	4.38578604913373
H	3.00895860055620	8.14269551879427	3.97580332037478
C	2.96001684879165	8.08556638834603	1.29108290430111

C	1.09744393481620	1.16416885892109	-0.78870681175721
H	0.28379550449309	-0.15333261855091	1.40567815029505
H	2.50458184022703	6.01346314695185	-0.37566361649891
H	1.85687444003829	3.73714931947997	-1.06498684944087
H	1.68564086925137	8.43225863268456	5.82499995414807
H	2.00708312561031	8.95872805529116	8.23340295967607
H	2.99753834361942	7.24891827049561	9.77305344519187
H	3.66245372696182	5.00939908413391	8.8746373237364
H	3.34545107932144	4.48488681938415	6.46554183381018
H	0.99007706616751	-1.39458824464094	3.17076030164299
H	0.00799771498437	-2.96380724752260	4.82798884558379
H	-1.48449108892839	-2.10302463428486	6.64528446811656
H	-1.97282582009761	0.35049646146861	6.78969239087096
H	-0.98344020464872	1.91920464522781	5.13604646129759
H	4.05384668649083	-0.46241197758012	7.37674384099037
C	2.99175768186103	-0.54217580034670	9.84164190713487
H	-2.39374574411410	5.94528206755942	7.88257434209221
H	1.27861302686756	1.16760626837044	11.01566671469762
H	-0.41968983353214	2.95110025673164	11.17100097271373
H	-1.48795044180219	7.55126276100976	6.52954992260499
H	-2.20794264962229	8.81879050593927	4.51749038661006
H	-2.39605267829907	7.66291663136387	2.30362556552227
H	-1.83597156185486	5.22805272672237	2.12610708967738
H	-1.09550067331703	3.96677963740779	4.13391514080662
H	3.82052936767685	-1.17388591002497	5.28745322750195
H	5.21095433816709	-1.44288494725600	3.24906543839888
H	5.91622284551080	0.56719012333221	1.93124039748478
H	5.19097749953085	2.84886148887124	2.67066904854117
H	3.77922814493313	3.11452476118418	4.69684480338398
C	4.35145518888257	-0.74951938449712	10.16819193600923
C	4.71386285922217	-1.65279043520230	11.17635214802668
C	3.72599230048732	-2.37335726283367	11.86669591106951
C	2.00582396859411	-1.27519427269365	10.54243104830186
C	2.37259879920087	-2.18511715077315	11.54359187911685
H	5.12376470621760	-0.17749728095031	9.64261421163936
H	5.77082369688151	-1.79142685081646	11.42568613179371
H	4.00983783146209	-3.08118256826071	12.65200871208446
H	0.95086788514046	-1.15426205641457	10.27486747853176
H	1.59825699747166	-2.75452699970235	12.06787896276080
C	-2.19071596867605	4.77933012696752	10.29238225738791
C	-2.87747795717556	3.75778675968932	10.98886027073736
C	-3.68297740566793	4.06638748600426	12.09366919669156
C	-3.81099616896096	5.39611481111700	12.52594665539822
C	-3.13595524736979	6.41926596798011	11.84114601233293
H	-2.80636560299218	2.72263831781934	10.63876068586274
H	-4.21907829333882	3.26563643551922	12.61331308334514
H	-4.43743293070393	5.63440351681667	13.39142378399106
C	-2.33785403350017	6.11524390233222	10.73016852470042
H	-3.22884498383635	7.45793095226609	12.17455970927494
H	-1.80046944168247	6.91331616618090	10.20659291834989
C	-0.04848302133338	0.53200560478177	-1.32274264733181
C	-0.03427962263157	0.00803160650204	-2.62246395439124
C	1.12749042361910	0.09536716141906	-3.40609823188592
C	2.27631330624088	0.70974192290522	-2.88240061216745
H	-0.96141687692708	0.47591575073351	-0.71993816943451
H	-0.93479586236416	-0.46677570417210	-3.02521629837369
H	1.13870082671688	-0.31667384519640	-4.42018765167640
C	2.26284624538185	1.24318462366717	-1.58614069192559
H	3.19039861128763	0.76797355916505	-3.48222969397576
H	3.17100544321705	1.69457393273165	-1.17306764515650
C	2.08200079850470	8.47908903292590	0.25455499761524
C	2.39935688876907	9.56475826631559	-0.57345132253914
C	3.59861922752523	10.27045282967903	-0.38567048065459
C	4.47662747991425	9.89088809642688	0.64223039124828
C	4.15820178699697	8.81195808952517	1.47792110964817
H	1.13130117218103	7.95204846893268	0.12233457914411
H	1.70294575662423	9.86459506469921	-1.36328255144619
H	4.85236137048453	8.50911043385186	2.26935968467566
H	3.84635231977251	11.11503401607226	-1.03651613355051
H	5.41492534816358	10.43461146520751	0.79235706527401

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Bis-tpo oxidized

Cu	1.23961702302938	3.37585407948489	5.15902337037833
N	1.86857292703287	4.95731716753082	4.10490232868238
N	1.08635809303445	2.51082033239633	3.36320294196361
C	2.27881929192512	6.17588650877118	4.53296035268459
C	2.60952588029703	7.18992534077335	3.60000778235815
C	2.54083693671405	6.99010867237947	2.21934291965832
C	2.19392102874673	5.66668447877946	1.76858650498039
C	1.85579046867783	4.69696043185701	2.75687205003445
C	1.48656987413767	3.35920856370468	2.36094697117792
C	1.53577719097186	2.97967844903763	0.98790519312414
C	1.17108189358107	1.62694031787793	0.65266285698813
C	0.70686237663681	0.82040762331483	1.69426403603938
C	0.66122449679205	1.26605963718943	3.03840711469844
C	2.21745368804487	5.25906499961056	0.39476884184359
C	1.89487728315526	3.97367187044821	0.01989209015964
C	2.41526291364194	6.45364235584620	5.98233665094704
C	2.04602637159009	7.71722351832791	6.50032716572768
C	2.24977927028118	8.01923911174264	7.85260782204938
C	2.84028301750770	7.07253538637021	8.70637763763858
C	3.21827735809668	5.81786421293327	8.20157180039421
C	3.00221766215782	5.50749782746513	6.85269690569530
C	0.10997025644491	0.36866274952194	4.08079780303289
C	0.40493701690651	-1.01451951275674	4.05658157679469
C	-0.18158195133552	-1.88323514591776	4.98545829499118
C	-1.08572806065942	-1.38909115677523	5.94043869867933
C	-1.39245224076890	-0.01898164234843	5.96836086848759
C	-0.79463998140324	0.85504454190679	5.05129914282079
N	1.92098595419587	2.04770952362336	6.48677047991104
N	0.09416170833711	3.99343472502102	6.68295147878072
C	2.88188516352645	1.10262978419837	6.34742683227269
C	3.19433141332461	0.23203296259190	7.42043996353183
C	2.55931132442322	0.31433192079805	8.66169086404417
C	1.60148614637805	1.37569017577272	8.83435959139199
C	1.30560777059318	2.19533446216395	7.70591835911489
C	0.33318817240495	3.25657170998681	7.81679040328947
C	-0.31738349405061	3.50068888157690	9.06204078515102
C	-1.30135654124945	4.55079150844021	9.10986593262300
C	-1.51369931163869	5.27511481452057	7.93416126057642
C	-0.82553439794832	4.98785906495215	6.72911869711093
C	0.99637487290005	1.70480127524193	10.09134266613266
C	0.07687688609927	2.72348668681103	10.20053834762008
C	-1.18765866853979	5.73405579409834	5.50060912422496
C	-1.44628374632135	7.12300768077501	5.56911544229691
C	-1.87640147456055	7.82432036975821	4.43581876206275
C	-2.07355739858852	7.14743175901193	3.22060106485141
C	-1.82752308889950	5.76706331345067	3.14235833569076
C	-1.38208123951718	5.06661085816916	4.27082903463499
C	3.64823001568101	0.98852529613787	5.08329049620459
C	3.97891262778733	-0.28664125420726	4.56797428086195
C	4.78138559619568	-0.40673916714617	3.42636006761808
C	5.28244171603600	0.74232050505382	2.79221383783984
C	4.96690739832676	2.01318971482849	3.29939443325543
C	4.15064821161448	2.13680156887606	4.43133358651538
H	2.92131535090972	8.16403761058059	3.98516114397713
C	2.84474533045232	8.10916614477011	1.29928878261909
C	1.24048854482762	1.08211819450982	-0.72200162706701
H	0.36870198587515	-0.19564246985883	1.47579116104263
H	2.51086775554381	5.98905190973609	-0.36330403959061
H	1.89816646368435	3.69862620348335	-1.03742314922075
H	1.57638891214065	8.45598853653559	5.84315487991138
H	1.95629505922205	9.00023347277467	8.23914375215788
H	3.01846041249214	7.31738216602989	9.75806214874212
H	3.70328762728805	5.08677932760623	8.85589703249403
H	3.34634711457992	4.54543047617591	6.46057501884349
H	1.11436066499638	-1.40422788961114	3.31962364949707
H	0.05985143367823	-2.95031077294962	4.95784669114920
H	-1.56116744251891	-2.07303361770933	6.65035896531574

H	-2.11826852390157	0.36653558319211	6.69126498799817
H	-1.07951275157543	1.91178838291784	5.04912930650480
H	3.96330595044512	-0.52779380157253	7.26029538512531
C	2.90416152065117	-0.64918012140770	9.73061062111890
H	-2.29840155159782	6.03505437117734	7.91038633777743
H	1.30250575913829	1.14893654838292	10.98090449217821
H	-0.34931459228820	2.96959649045823	11.17577597806697
H	-1.28972944591923	7.65608989523269	6.51232682589652
H	-2.06868136257537	8.89958261435322	4.50323522517063
H	-2.43335718024544	7.69198318919080	2.34208043509352
H	-2.00652626437059	5.22968460831703	2.20575403525201
H	-1.23927025965877	3.98313872042710	4.21112612352981
H	3.58682749904501	-1.18548104605496	5.05454042727810
H	5.02503797006631	-1.39994954072938	3.03661168361551
H	5.92955594393175	0.64605151776862	1.91485047851765
H	5.37700892000634	2.91072305612918	2.82574575715251
H	3.95101083721807	3.13017841721847	4.84518493488299
C	4.26056061306299	-0.96974451913896	9.98115608810302
C	4.59881792612314	-1.90522724314932	10.96594220206521
C	3.59073455677852	-2.55143169620509	11.70111294701853
C	1.89659638935381	-1.30605050641311	10.47924076315334
C	2.24059517182458	-2.25449383577285	11.45045769128928
H	5.05079440269480	-0.45252808383843	9.42656787701783
H	5.65171956360092	-2.12823536454161	11.16362301879102
H	3.85676111874952	-3.28702117417172	12.46637753308867
H	0.84186513862701	-1.10446413169835	10.26550436573823
H	1.45256847058991	-2.76891894278626	12.00904496975217
C	-2.0968338889198	4.86405341174364	10.31897589338288
C	-2.75657950769448	3.84797467685083	11.05227734733296
C	-3.54942648712955	4.17472304077463	12.15990564466404
C	-3.68494665702085	5.51367734614993	12.56166060488916
C	-3.03587931485274	6.53027038362007	11.84117592044302
H	-2.68682465308543	2.80591058993550	10.72362970126913
H	-4.07052809791093	3.38223734925334	12.70581083181599
H	-4.29947379264756	5.76517024375460	13.43146007071367
C	-2.25738579302912	6.21107170032472	10.72222494713308
H	-3.13600230611080	7.57434841105654	12.15328633961528
H	-1.73944441103644	7.00434664536269	10.17259403664526
C	0.15129516291337	0.34137062050389	-1.24153972983308
C	0.21627735729626	-0.20944878196685	-2.52687532550398
C	1.37516326067445	-0.04982910762566	-3.30512843041033
C	2.46960816921055	0.66756735672012	-2.79371364940103
H	-0.76215803692927	0.23231311402539	-0.64716554344655
H	-0.64064981173862	-0.76192020043621	-2.92421986567099
H	1.42659203806186	-0.48644027187174	-4.30722827832874
C	2.40369620403980	1.23671530965697	-1.51582216385306
H	3.38065132912765	0.77792642926551	-3.38991453287643
H	3.27344014091766	1.76372275150627	-1.11008174326689
C	1.98638984589826	8.42322977652722	0.21676758404452
C	2.26229673454114	9.51872705305022	-0.61085322434675
C	3.40251775418655	10.30729948490569	-0.38266948661988
C	4.26092629202671	10.00526437207365	0.68787726249686
C	3.98052494523393	8.92258100921357	1.52991966641347
H	1.07724410818239	7.83495117163396	0.05495865956971
H	1.58165822355098	9.76251351826215	-1.43240250475684
H	4.66407509192855	8.6785582275686	2.35017792959458
H	3.61994851219797	11.15772470510089	-1.03610547884107
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Bis-tpg triplet

Cu	1.23388333920444	3.37332250577458	5.15819164014767
N	1.82244008140144	4.95832484313356	4.11890696335499
N	1.11117976759829	2.49756274794704	3.38158150495867
C	2.25504372646642	6.17512983707771	4.54807596689738
C	2.62124967211622	7.17517132758186	3.62472652046914
C	2.56887628041969	6.97235280295728	2.23398520124220
C	2.21221898518599	5.66223173234415	1.78124504426750
C	1.84972458317934	4.68759434087097	2.76191277227039
C	1.48417427578851	3.36201450339178	2.36777463995155

C	1.51744509352792	2.97718193477981	0.99143415975539
C	1.14256972358985	1.63661531954178	0.65790238383014
C	0.68252970772714	0.82168321331063	1.70762156911948
C	0.66596303626183	1.25624565982035	3.04838461686154
C	2.23312608612783	5.25142029319937	0.40586385934627
C	1.88820746511373	3.97419322114012	0.02755922415080
C	2.38007818863195	6.45732131164197	6.00066173115029
C	1.99884183857244	7.71818847828701	6.51529850471292
C	2.19691044541436	8.02826183212601	7.86726215481868
C	2.78847929114044	7.09000783362461	8.72835545680253
C	3.17593423750605	5.83619421872535	8.22817009415967
C	2.96943589812191	5.52083353809573	6.87925364945062
C	0.11842192061094	0.35272723480180	4.09161244983620
C	0.42219553127220	-1.02806329523084	4.06903084393182
C	-0.16249402014767	-1.90358366723584	4.99359214232170
C	-1.07022439610005	-1.41892781177731	5.94893704973177
C	-1.38423000802503	-0.05031568321791	5.97764106910167
C	-0.79158456014220	0.82813269735645	5.06195450745104
N	1.89379041787256	2.03343888441768	6.46154971917011
N	0.10818541536560	4.00499219711636	6.67246921912557
C	2.87698348269518	1.10132367666643	6.33187142950279
C	3.21138628111601	0.25314707884827	7.40629011726145
C	2.57489511980207	0.33549379425598	8.65771136513477
C	1.60972414003585	1.37870219299860	8.82776023061271
C	1.29567939251336	2.19690180188044	7.69851448597931
C	0.32810605001245	3.24600703694817	7.80806004619625
C	-0.34335836269914	3.48649399674355	9.04735298804915
C	-1.32394750752063	4.52752239392745	9.09029646435618
C	-1.53935646633145	5.25495905799197	7.90655611070759
C	-0.83643507020451	4.98223285788069	6.71449177178867
C	0.99008339947041	1.70393847537759	10.08155345355680
C	0.05323099507112	2.70576978195586	10.18523848473857
C	-1.20011511707493	5.72944845616934	5.48362249427430
C	-1.45786613607395	7.11819001339710	5.54859543607601
C	-1.89256703671693	7.81896271492589	4.41596680411343
C	-2.09015866954572	7.14354506628956	3.20086099232303
C	-1.84286065103558	5.76316468912418	3.12488295503108
C	-1.39728275467509	5.06390690894414	4.25361746706430
C	3.64583444579042	0.98937537488028	5.06605510112195
C	3.97596992524895	-0.28329395792674	4.54545397255492
C	4.78391903316405	-0.40234344888610	3.40683278103256
C	5.28738792426106	0.74595443959663	2.77488111732025
C	4.97074107397925	2.01542204852532	3.28560563398704
C	4.15330522212298	2.13654953332804	4.41639097164817
H	2.94286375540004	8.14475682911159	4.01312601155822
C	2.90554560858347	8.08990949830229	1.31963051978348
C	1.18959961450627	1.09338269451235	-0.72104620702000
H	0.33412466003791	-0.19058317736688	1.48784551566363
H	2.53693132728023	5.97788077800039	-0.35196129331483
H	1.88901029822338	3.70344997258046	-1.03118293202781
H	1.52360463790612	8.44751779088857	5.85157416950028
H	1.89017379884780	9.00769145648687	8.24881885193894
H	2.95233039239334	7.33620327607694	9.78232897210437
H	3.65256378869579	5.10443758669999	8.88818046574100
H	3.30404349010650	4.55184893646268	6.49623552164338
H	1.13924915288036	-1.40801255794128	3.33431909389195
H	0.09059643188751	-2.96843813851065	4.96644833080878
H	-1.53572648025286	-2.10556650867500	6.66324820474883
H	-2.10477441004033	0.33359483666953	6.70695570061866
H	-1.06773589237720	1.88699550389847	5.07416088945461
H	3.99152349758625	-0.49579850222869	7.24900807896336
C	2.94287076580505	-0.61793245878269	9.73111805277063
H	-2.32944421664499	6.00921253980075	7.87928440423525
H	1.29615611376465	1.15179282621567	10.97385854709785
H	-0.38363121691529	2.94175579109075	11.15870053993796
H	-1.29410559692064	7.65035802810880	6.49113440803297
H	-2.07983283908267	8.89558522143053	4.48310504931180
H	-2.44189194560131	7.68904913311509	2.31934266172886
H	-2.01043981953908	5.22501195518049	2.18642194673518
H	-1.23472886579102	3.98369171075917	4.18890121601928

H	3.57611145458732	-1.18073317656878	5.02833962970968
H	5.02264142064458	-1.39573724224740	3.01323053750510
H	5.92899925410388	0.65182010805354	1.89292266985158
H	5.37252188786030	2.91575074362589	2.80974166183040
H	3.93766048926664	3.13029297502463	4.82103183934981
C	4.30440183018546	-0.90897080059523	9.98534405028769
C	4.66621090658162	-1.83499385166883	10.97187486425303
C	3.67651316937865	-2.49814033374897	11.71570238305919
C	1.95548320111687	-1.29665453574991	10.48544370203325
C	2.32119122272537	-2.22870437467125	11.46573697576357
H	5.08121628292585	-0.37940383221527	9.42327128754512
H	5.72512069807129	-2.03583689387502	11.16427668369332
H	3.96012763485561	-3.22390493989169	12.48449728907578
H	0.89655419577626	-1.11763266526373	10.27239227092069
H	1.54370959790659	-2.75371782303590	12.03028536943489
C	-2.12318314637622	4.84722834585466	10.29828350935542
C	-2.79504775945239	3.84046613062946	11.03172635605686
C	-3.58178945429238	4.17197731312535	12.14316907394923
C	-3.70962121252361	5.51102829793290	12.54565540410738
C	-3.05310429868652	6.52045729850848	11.82282980748552
H	-2.72964893213980	2.79794507120527	10.70352917200735
H	-4.10555656815947	3.38154413339494	12.69054731355485
H	-4.32228547767409	5.76743284617641	13.41576677819998
C	-2.27330736442728	6.19344742505257	10.70615635280939
H	-3.14622604425047	7.56663626136314	12.13195732433948
H	-1.74923434104106	6.98148387421961	10.15466302282496
C	0.08389728239133	0.37705800473260	-1.23736215043007
C	0.12642632240538	-0.17409852724073	-2.52444988350458
C	1.27772619715963	-0.03242070135801	-3.31611660458287
C	2.38767924598905	0.66408942820620	-2.81117323073083
H	-0.82375526396997	0.28026721317653	-0.63183386741437
H	-0.74443568015503	-0.71239183428015	-2.91240009536667
H	1.31122996159125	-0.46604394147064	-4.32063914917234
C	2.34575966767639	1.22423161316546	-1.52737231716481
H	3.29497081753764	0.76403712252556	-3.41585738472214
H	3.22774668483678	1.73477096396004	-1.12701307136428
C	2.06657458616521	8.43250034215931	0.23197362449833
C	2.37781681516148	9.52054158014918	-0.59440473610092
C	3.53193925383640	10.28392361958352	-0.35494531607305
C	4.36988900134057	9.95818197561127	0.72396407502596
C	4.05759425468002	8.87645794851570	1.55738424494032
H	1.14631731882208	7.86447783634567	0.06067096780778
H	1.71065110435070	9.77883436284247	-1.42325659081171
H	4.72528496805364	8.61488893628806	2.38541264236682
H	3.77513005039054	11.13116256999575	-1.00398975222539
H	5.27349197682641	10.54614007512639	0.91492921327573

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Bis-dmpp reduced

Cu	1.36694634138631	3.31648702723612	5.20692653059037
N	2.06090632452935	4.84984112834666	4.08693436970800
N	1.14103302976000	2.38482378692340	3.41942059613041
C	2.44637356998829	6.10104532839166	4.44282990681128
C	2.79408651046716	7.06899290377689	3.45774434165179
C	2.76526077376040	6.74795346428998	2.11144947441298
C	2.36856612152870	5.44579673099478	1.71531479372021
C	2.00462807355117	4.53338369707334	2.75130550302121
C	1.55976888239851	3.20406003057872	2.39935970049164
C	1.56873992686066	2.80531486649191	1.02837411335984
C	1.15732690836129	1.47992193104387	0.73890147074413
C	0.76265725310840	0.65018927944964	1.77408489032266
C	0.75033947056968	1.12073669204305	3.11850078835933
C	2.33904977801030	5.02028784695821	0.34510286920900
C	1.96596711720285	3.73974087336435	0.01429522616920
C	2.55662362941113	6.46230643947579	5.87593595362818
C	2.25396299080810	7.77614796076029	6.30410593522996
C	2.41614853177124	8.15019738071009	7.64187324754386
C	2.90514881910152	7.23932120395345	8.60159362316284
C	3.19981591007438	5.92903449506463	8.17210484035505
C	3.02144229211489	5.54207989984261	6.83953400067907

C	0.25477157138790	0.22145816893688	4.18759714828496
C	0.49504276582102	-1.17074676128010	4.11574104398376
C	-0.02447022606212	-2.03950063251650	5.08084113207544
C	-0.82034298762826	-1.56146253268804	6.14275596994345
C	-1.05184960962707	-0.17235118619624	6.21505365626002
C	-0.51898123404367	0.70448208651848	5.26428447871875
N	2.13455185447725	2.11256095231229	6.64645870573749
N	0.10592182271997	3.91441743139718	6.67117631036501
C	3.1019189677866	1.16276466497585	6.58814418216356
C	3.41680502230547	0.36691954007281	7.72694083208285
C	2.75249096672676	0.55551588394714	8.92652625191577
C	1.73776968622777	1.54183402079559	9.01177208491402
C	1.45341471049447	2.28572674302627	7.82685216040944
C	0.40480659643356	3.27989074457057	7.85206605420664
C	-0.27035820580506	3.55387903774372	9.07980386209502
C	-1.26417106484245	4.56481209333381	9.05872117398066
C	-1.54167887199869	5.21994093581378	7.87099425976196
C	-0.85231218863569	4.87463747043122	6.67380711139407
C	1.02022994025785	1.82325086886899	10.22232958835801
C	0.05971023453002	2.80541485781223	10.25890480242432
C	-1.22760238692076	5.54717893035672	5.40764598094530
C	-1.59887616582646	6.91152587232422	5.40913453150108
C	-2.01665341873681	7.54252096416679	4.23242563316135
C	-2.10166958192385	6.83635790119443	3.01481227791340
C	-1.72586392381911	5.47678532593794	3.01676274815115
C	-1.28853974938246	4.84424059365842	4.18508003865895
C	3.88295906043508	0.97314235351767	5.34271870880302
C	4.3504257702474	-0.31296811601097	4.98362895384171
C	5.14504127626017	-0.49670773712335	3.84761548149666
C	5.52357352157262	0.59291683705016	3.03563606297261
C	5.04937520799140	1.87206444911538	3.39214026168023
C	4.23809082321271	2.06017135519618	4.51606236257278
H	3.13942703622386	8.05281306074674	3.78410860311223
H	3.06327025949778	7.47988620053422	1.35320932751577
H	1.13708720638672	1.13108714017173	-0.29908183906963
H	0.40062743606568	-0.35921553628542	1.56524224708762
H	2.62997985199977	5.73567946611335	-0.43130177259750
H	1.95672865407608	3.41289889000327	-1.03084987042208
H	1.85634267557808	8.50312000192326	5.58824079686759
H	2.16030671579182	9.17064134422279	7.94909225127853
C	3.13255935211225	7.66399082325983	10.03433449695411
H	3.58541377236079	5.20139946949984	8.89520244583083
H	3.26581550321734	4.52081291339355	6.53567783906723
H	1.12337140531926	-1.57399994353864	3.31479437913962
H	0.18982356338732	-3.11188186244056	5.00896681225756
C	-1.42710957476450	-2.50981825999589	7.15134857091737
H	-1.66866805548558	0.22755833595499	7.02786860287565
H	-0.71595022632591	1.77659781851110	5.34514942458171
H	4.23169245588826	-0.35718998874011	7.65531799592920
H	3.01467311372246	-0.03311440177996	9.81211071935278
H	-1.81539416265118	4.80461372654539	9.97421457793260
H	-2.33411349909634	5.97082783220794	7.82532605418426
H	1.26197232946760	1.24471377429380	11.12016268416348
H	-0.47700011917064	3.02770064845967	11.18720459284491
H	-1.52876818448188	7.49293147167508	6.33445136107834
H	-2.28507242759340	8.60474011239866	4.25855821958244
C	-2.60805640980581	7.50482778350942	1.75716005692711
H	-1.78702989688794	4.90161855896777	2.08584685115595
H	-1.01479752541743	3.78624416343678	4.15735786470694
H	4.06076905963613	-1.18385058306450	5.58073139886311
H	5.48068077199611	-1.50634836005871	3.58477515188590
C	6.42865959661831	0.39780627954945	1.84086699511890
H	5.32865638273510	2.73781603417330	2.78101992477361
H	3.88402137849281	3.06342217130803	4.76702852455156
H	6.27749928263043	1.18443647235204	1.08268923004937
H	6.26282670934129	-0.58163039936308	1.36085525959404
H	7.49275593104040	0.43462726663844	2.14180694978838
H	2.38536042067532	8.40686359655582	10.36174609173874
H	4.12778085903923	8.13247330076038	10.15368259031245
H	3.09191150964921	6.80519800950475	10.72513332814703

H	-2.14178937173030	7.07792443621288	0.85301830072297
H	-2.41386676036419	8.59049455714018	1.76677793317572
H	-3.70135884929613	7.37077366608761	1.65230518068612
H	-0.78379305027659	-3.38994583662537	7.32030483995765
H	-2.40590190155338	-2.88685242929402	6.79911749903437
H	-1.59956710946755	-2.01588171595480	8.12238563892457

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Bis-dmpp oxidized

Cu	1.37157890611620	3.30337727188601	5.20520518374401
N	1.96241529625996	4.86121836752641	4.08305897421805
N	1.24152783246848	2.33552454647326	3.44741860054217
C	2.33464165604082	6.11115648105795	4.45242856727984
C	2.67117973485150	7.07901994875166	3.45810424755207
C	2.66321910159037	6.75012058115027	2.11545191523569
C	2.32400399984701	5.42827135232557	1.71816060681104
C	1.97109367549289	4.51635846990092	2.75399904473392
C	1.61124165430783	3.16554122715105	2.41824593182693
C	1.64365371691973	2.74631550594894	1.05711860740241
C	1.28424788224420	1.39686527627049	0.79270708555043
C	0.89341468104644	0.57727661048246	1.83510292511120
C	0.85334532301524	1.06546750007699	3.17612401486313
C	2.33878796872418	4.98168410598724	0.35505171659232
C	2.01143757343389	3.68352613098158	0.03536286668667
C	2.45593366261896	6.46942162899158	5.87876686815234
C	2.09708952351493	7.76561200386849	6.32263617406473
C	2.29424150711596	8.14411478588636	7.65275974118406
C	2.88252900320560	7.26192206914151	8.58738250682773
C	3.24007761157077	5.97174818310328	8.13979644986551
C	3.02668171855078	5.57713595024864	6.81536173204894
C	0.32804757964566	0.19523421811992	4.24594516956200
C	0.61951309875003	-1.19058696520033	4.24852767545799
C	0.05250961425085	-2.03659171959804	5.20479827216012
C	-0.84890135047447	-1.54588362654117	6.17665498606138
C	-1.13829929391845	-0.16424293526036	6.16804412075459
C	-0.55888790470869	0.69345674834479	5.22781266251599
N	2.07065943888904	2.03886488299450	6.59935198933131
N	0.19231786445174	3.97868610359970	6.68681956338302
C	3.03427968966252	1.08982863432522	6.51092614276889
C	3.33133649770991	0.26617112918117	7.63851512811375
C	2.67737356348102	0.44887285217856	8.84282469256959
C	1.70161959848283	1.47532099783743	8.96360194465913
C	1.42896930663142	2.24384585174680	7.79563371214755
C	0.44722372190243	3.29271099689696	7.84852404168622
C	-0.21674371956231	3.57332073647159	9.07711194081916
C	-1.16969698869971	4.62777715155943	9.06477753074269
C	-1.43308770406292	5.29658387899928	7.88389224526174
C	-0.75461292994684	4.94844062520475	6.67684356966716
C	1.01067141456713	1.77322117426338	10.18494177005739
C	0.08409978872348	2.78963041101156	10.24034410118514
C	-1.13976296702460	5.61026969720778	5.41539445070108
C	-1.46785296901750	6.98786821301310	5.40202793296118
C	-1.92240936483650	7.60115449044877	4.23208240026943
C	-2.09789185138568	6.86521782424867	3.03813479474870
C	-1.77164559070734	5.49195086571214	3.05732561415273
C	-1.29554032774532	4.87444126060278	4.21816385305409
C	3.82581396648081	0.93733508523871	5.27491045921255
C	4.22355258741810	-0.34854724279343	4.83484468691624
C	5.04633740233383	-0.49585927035165	3.71551233187777
C	5.53080083746495	0.62759371782477	3.00763013364676
C	5.13445195246980	1.90724213808115	3.45269179396298
C	4.29384344381800	2.06339333313523	4.55928871777555
H	2.98446975222318	8.07322526527044	3.78501983008487
H	2.94182284632096	7.49038116189850	1.35818323147472
H	1.29315480745403	1.02393069397127	-0.23681128842559
H	0.55916747410480	-0.44503826884783	1.64359240850573
H	2.62094558192605	5.69328152965071	-0.42722631841868
H	2.02218728861923	3.34716313083736	-1.00611958268241
H	1.63325685947299	8.47050772241739	5.62501011202144
H	1.99903895896440	9.14883626604233	7.97422678693099

C	3.15827312466341	7.70418989779021	10.00350513488852
H	3.71990019479173	5.27711646091397	8.83791709040790
H	3.36810100701298	4.58901362127010	6.48995335448926
H	1.31891735876268	-1.60081293246949	3.51280365924577
H	0.30135693442675	-3.10330146832937	5.19278656981607
C	-1.51226678943582	-2.47897902044406	7.15976922815700
H	-1.85301801646702	0.23720729795384	6.89478066978167
H	-2.84953727524659	1.74899558812580	5.21438391861911
H	4.12397147796647	-0.47960748475152	7.54324141441896
H	2.92359937460696	-0.17147645896225	9.71092320683344
H	-1.70770590301755	4.88468926142340	9.98325688787487
H	-2.20317323114147	6.07045755716108	7.84322766925229
H	1.23870311325708	1.17892503828426	11.07531119802620
H	-0.44200267511812	3.01270226225209	11.17383181407183
H	-1.33716658837540	7.58697422037583	6.30907361263869
H	-2.16007740138666	8.67041122880381	4.24399493406610
C	-2.65828774358989	7.51994855964793	1.79940021366214
H	-1.92205894593397	4.89350544328758	2.15210870195482
H	-1.10661035137320	3.79593346651705	4.21219280648877
H	3.85979848791932	-1.23903347391171	5.35778305338483
H	5.33195246797069	-1.50135727624845	3.38785300513233
C	6.47599283185426	0.46102462766281	1.84307841154474
H	5.51652424756376	2.79533421895656	2.93744221983495
H	4.05412019526423	3.07216107324907	4.91134500682587
H	6.47490069399757	1.34401291545114	1.18341512101349
H	6.22553796315035	-0.42781333083182	1.23981205945501
H	7.51306670312034	0.32212391677919	2.20238952447167
H	-2.40705000997236	6.95536031228012	0.88674895343551
H	-2.29186963310436	8.55397285199753	1.68398947687227
H	-3.76170921099277	7.57613988441187	1.85623905795316
H	2.35662346457512	8.35590289998845	10.39006182489289
H	4.09630884215318	8.28879603246159	10.05103076147670
H	3.27306212497763	6.84703106107597	10.68679857075509
H	-0.82603766835695	-3.27631945932207	7.49162242805521
H	-2.38162654591325	-2.97925559512429	6.69298807182474
H	-1.88293662167365	-1.94335995468020	8.04889300041000

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Bis-dmpp triplet

Cu	1.36874367072601	3.30286643109810	5.20439355374194
N	1.93134447641239	4.86027302359369	4.09719620617250
N	1.26647479830478	2.32833527860290	3.46866657234089
C	2.33120165602186	6.10896606023679	4.46477766836335
C	2.70308112038891	7.06221192887130	3.48455560536207
C	2.70054036208076	6.73533057736378	2.12840869848328
C	2.34799241591553	5.42601386155796	1.73141928803670
C	1.97209288282188	4.50763166131502	2.75945445076319
C	1.60922494753600	3.17100372355624	2.42576935072730
C	1.61840862512557	2.74465909700328	1.06190347464961
C	1.24568970572224	1.40777304118990	0.79752008978684
C	0.85511912568787	0.58424848124454	1.85349324845184
C	0.85277000047842	1.06195644014303	3.18750534874166
C	2.35276547843761	4.97463040630702	0.36718409005791
C	1.99618584226465	3.68637532446413	0.04450400936703
C	2.43959015779682	6.47053035336984	5.89723431921931
C	2.05598165733784	7.75729718516224	6.34105917840327
C	2.24089540247980	8.14063949602005	7.67367063953958
C	2.83130007031230	7.26797010789865	8.61159089667244
C	3.21351486319992	5.98574360956447	8.16537199903136
C	3.01860373094116	5.59018716766339	6.83801112912925
C	0.33750619466650	0.18510677596601	4.26466000552531
C	0.65103569508739	-1.19346068090664	4.27708542033825
C	0.09516457164731	-2.04605525487045	5.23728661576034
C	-0.80779189249704	-1.56567566687857	6.20827531180015
C	-1.12005196857737	-0.19000858800266	6.19145519045897
C	-0.55720853283082	0.67094800402289	5.24404804713104
N	2.04977347147654	2.02801682685868	6.57494880193750
N	0.21789247270424	3.99694000262330	6.67612219103912
C	3.03546266216347	1.09186308083015	6.49915204316016
C	3.36161581678541	0.29787136686859	7.62638879144776

C	2.70807536184600	0.48043165676838	8.84543816081827
C	1.72643643999642	1.48994403366199	8.96153284286318
C	1.42823169764773	2.25308813281054	7.79088629303382
C	0.45070442968975	3.28791726508281	7.84166827759988
C	-0.23597997163374	3.56650421662022	9.06334372843616
C	-1.19460267237368	4.60421368322308	9.04658591688088
C	-1.45445337291868	5.27713104068927	7.85240840095146
C	-0.75217249694438	4.95222596736957	6.66546417638770
C	1.02537575293579	1.78911745249052	10.17972913056542
C	0.07741668268510	2.78420208163477	10.22728096232025
C	-1.12807828204800	5.62378628816094	5.39971018040976
C	-1.42545552167640	7.00611985362467	5.38365042679558
C	-1.87033820601158	7.62956881329155	4.21293376831756
C	-2.05555238024606	6.90030707232796	3.01975471544669
C	-1.75952025758418	5.52141488753996	3.04004732978351
C	-1.30028380033009	4.89388704416059	4.20269021212383
C	3.82053236070288	0.93150889540368	5.25322390703012
C	4.19464209505881	-0.35581973243032	4.80345576098638
C	5.01086824374103	-0.51221586528625	3.67810712565657
C	5.50234337090612	0.60375679020180	2.96889758622928
C	5.12959239880688	1.88626023851689	3.42229848225121
C	4.30195760532023	2.05031932797287	4.53791729190059
H	3.03165419797415	8.04921814836257	3.81816324240465
H	2.99417610039155	7.47370789457175	1.37523167152593
H	1.23951640354995	1.03628604544416	-0.23237622558499
H	0.50389582244983	-0.43294332511375	1.66528906328427
H	2.64612898594451	5.68265070889389	-0.41505068000074
H	1.99646681577195	3.35438006481912	-0.99906023191397
H	1.58184412760175	8.45016639840064	5.63826028609460
H	1.92256166180691	9.13923469377301	7.99410575371380
C	3.07702175313027	7.70515714049493	10.03748590143049
H	3.68424723258712	5.28997592482267	8.86899558557227
H	3.35455628696275	4.59802235587712	6.52023410317669
H	1.36045424296682	-1.59113695886395	3.54403233910444
H	0.36522887657822	-3.10821471471296	5.23306343675808
C	-1.44655742739913	-2.49869964797499	7.21143057625960
H	-1.82739202143467	0.20960329389076	6.92687160091363
H	-0.84424498018231	1.72729479812931	5.24162872923557
H	4.16673670863587	-0.43428032284901	7.53040118255390
H	2.96800134132324	-0.13089779341155	9.71572619144418
H	-1.74423376613846	4.85448075178745	9.95981506861235
H	-2.23486884778424	6.03998717280916	7.80215523352854
H	1.26185625447427	1.20365494778886	11.07447532388649
H	-0.45578909596801	2.99968829690542	11.15921687942415
H	-1.27669992169401	7.59932396583956	6.29183763134427
H	-2.08123728092463	8.70502270173955	4.22403197287390
C	-2.58670947392504	7.56744359869282	1.77170992202090
H	-1.90469850384341	4.92698168712000	2.13098269103234
H	-1.10959569022624	3.81597523642575	4.19047752570613
H	3.81536984205324	-1.23993900869842	5.32625376362360
H	5.27501528202159	-1.52153103964668	3.34235640430853
C	6.42475336830119	0.43076926061423	1.78391096211755
H	5.50589385367636	2.77217901642523	2.89851443873422
H	4.05802252263100	3.06118221529565	4.88011852747064
H	6.34738072208902	1.27710955535693	1.08092041315039
H	6.20606344363669	-0.49865216309321	1.23137062675048
H	7.48041500535158	0.37313671636704	2.11023748360355
H	-2.24737085847239	7.05098860807232	0.85812531100711
H	-2.27167576707727	8.62281532240102	1.70936706191003
H	-3.69306993162611	7.55822220910820	1.75961489666200
H	2.30685279930544	8.41524307503319	10.38332017272245
H	4.05403357805577	8.21601520818771	10.13098341931406
C	3.09140765270196	6.84672180058812	10.72985180677882
H	-0.80512314256853	-3.37109669616273	7.42097814215562
H	-2.41023085942664	-2.88728634832112	6.83116571489076
H	-1.65751627146980	-1.98750906176296	8.16598916797065

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85

Bis-dpp reduced

Cu 1.37245398432253 3.30706572064291 5.20686405578096

N	2.05853304051330	4.84162408429926	4.08296011578564
N	1.14197915036057	2.37415814925316	3.42358567287196
C	2.43993337956635	6.09527477083357	4.43249721475416
C	2.79741005455480	7.05680430286823	3.44574669812962
C	2.77999032286290	6.72719727221516	2.10086518497658
C	2.38367690741673	5.42356066627647	1.71000485049285
C	2.01101113616121	4.51766518369684	2.74865111118154
C	1.56746958652051	3.18707957643754	2.40120916132037
C	1.58243551630401	2.78011368245702	1.03279348235094
C	1.17226861221654	1.45341294071814	0.74845192775427
C	0.77306999118414	0.62887429788458	1.78704228225241
C	0.75456727082562	1.10887853393733	3.12704447993288
C	2.36165041610201	4.98984720459267	0.34169898401316
C	1.98745805919919	3.70863588666121	0.01568638123798
C	2.53149001016706	6.46701517890082	5.86638850974092
C	2.19904856573254	7.77879464789479	6.27844043976751
C	2.33929098755813	8.16437604559788	7.61777323994268
C	2.82836763802658	7.25215860040186	8.56683054275035
C	3.16256973845402	5.94746055382582	8.16908922326734
C	3.00624596858565	5.55512203972270	6.83369751645912
C	0.25969560011206	0.21665215725428	4.20497212191069
C	0.54217503084089	-1.16861170965650	4.16121872062095
C	0.02944939701308	-2.03358715690333	5.13656536460584
C	-0.78665198395051	-1.53345654607992	6.16410963782360
C	-1.07439343449061	-0.15996612116738	6.21712570392407
C	-0.54829341429498	0.70859692470952	5.25253884527996
N	2.14642927784077	2.11056798500691	6.63892157460539
N	0.11027307966883	3.90251225742393	6.67146678294500
C	3.11702287332081	1.16514619852388	6.57656464388762
C	3.43734201221663	0.36579573262509	7.71022503692291
C	2.77187543332265	0.54516754958942	8.91119630395232
C	1.75082951918754	1.52436226866773	9.00032720485716
C	1.46289629838766	2.27327031779383	7.81960000550002
C	0.40935467450175	3.26167099207484	7.84892779275333
C	-0.27183229629961	3.52241503799282	9.07616332551070
C	-1.27217328383009	4.52677285933774	9.05923888267325
C	-1.54773068653656	5.19082169731985	7.87547229731171
C	-0.85065997329899	4.85874288531923	6.67972532581139
C	1.02812175910877	1.79334412585401	10.21117190559807
C	0.06023800720744	2.76782945562970	10.25136424108819
C	-1.21846906452340	5.54432986668551	5.41581358829508
C	-1.57117591735931	6.91390931493072	5.43223475454726
C	-1.98091535991617	7.56017395279221	4.25886913997695
C	-2.06136376348854	6.84654547229371	3.05220849790495
C	-1.71491817232329	5.48583657587524	3.02439398627787
C	-1.28686485080182	4.84259347255334	4.19268756085677
C	3.89249797570361	0.98192477030821	5.32442322287016
C	4.33558786895849	-0.30887671633158	4.95166998392082
C	5.12304631859108	-0.49225199729607	3.80793271625854
C	5.49483965274115	0.61148247750420	3.02337715435844
C	5.05982036204952	1.89744621051966	3.38264583183759
C	4.25733377919674	2.08020695894478	4.51583615512039
H	3.13964488782741	8.04263818701611	3.76937937578692
H	3.08497677213644	7.45433704730780	1.34087044716694
H	1.15833399175696	1.09858917919287	-0.28750867821515
H	0.41469408849233	-0.38309558969850	1.58388889147255
H	2.65870332305962	5.70011042082250	-0.43698020860614
H	1.98382371022251	3.37619679757423	-1.02763384345437
H	1.80204770569251	8.49202734519822	5.54869680609244
H	2.06819937480321	9.18095441764591	7.92034613629607
H	2.95246817188056	7.55839774037022	9.61052164483802
H	3.55596360920592	5.23383603172480	8.90012853516918
H	3.27763491627334	4.54143100943087	6.52814028848260
H	1.19050451559507	-1.56541331127620	3.37320976661688
H	0.26601454882974	-3.10156152556666	5.09223327783740
H	-1.19956296201809	-2.21184683686714	6.91758496566309
H	-1.71909719047400	0.23631086114884	7.00820244345440
H	-0.78175363106971	1.77551828967770	5.29365062602432
H	4.25493101378413	-0.35495729291784	7.63432664222017
H	3.03700315407570	-0.04672556146616	9.79363282704490

H	-1.82841513152638	4.75595479922965	9.97433203304982
H	-2.34227085365037	5.93952822063015	7.83216183883024
H	1.27143450100520	1.21073064394676	11.10581182770996
H	-0.48073010198802	2.97974539542474	11.17951221576929
H	-1.49738224485500	7.48149432222746	6.36559071426694
H	-2.24149299208725	8.62307041731091	4.28788442576464
H	-2.39728180511386	7.34751745679993	2.13862407354247
H	-1.78925749402931	4.91962635168565	2.09036289575551
H	-1.02960023409091	3.78045705488287	4.16736880629208
H	4.03786519892337	-1.17802477817465	5.54713076576876
H	5.44948422458037	-1.49965818720468	3.53041782298101
H	6.12355451240810	0.47034597775182	2.13835774846353
H	5.35458746537264	2.76435424819057	2.78261685822355
H	3.92596789948773	3.08442425876768	4.79292864512160

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Bis-dpp oxidized

Cu	1.37519394986573	3.30646430011260	5.20701480981805
N	1.96082199001519	4.86466023068454	4.08322002235502
N	1.24195850018406	2.33936648530117	3.44740651811981
C	2.34231368794384	6.11067330745853	4.45377003219568
C	2.69612504148542	7.07474066590626	3.46352357029913
C	2.68940412816105	6.74680099918349	2.11967950878383
C	2.33805839587927	5.42911906606380	1.72052579509973
C	1.97515015900011	4.51879557450269	2.7545193434608
C	1.60764582652807	3.17054044506770	2.41762377394637
C	1.63041170028870	2.75370239826578	1.05555843487879
C	1.25574372184968	1.40917295143470	0.78946389030312
C	0.86272115245485	0.59019364322688	1.83274977060639
C	0.84227800241423	1.07386970468850	3.17490165066893
C	2.34823995839914	4.98347088998779	0.35634810564611
C	2.00581326891573	3.69001199912617	0.03476766385136
C	2.45229110480763	6.46923371408101	5.88443459279643
C	2.05678380423000	7.75519292676926	6.32419790219278
C	2.23648890781310	8.13468237253513	7.65994089789999
C	2.83355968248740	7.24706231227827	8.57158047403761
C	3.24125457653380	5.97276041303653	8.14334680705557
C	3.04526187873019	5.58238798512056	6.81272318666184
C	0.32881809439296	0.19936597800282	4.25165104625498
C	0.65309085659732	-1.17837008080179	4.25980052065818
C	0.10520846411344	-2.03066198425954	5.22620747542153
C	-0.79108758989697	-1.52699251563677	6.18455312793800
C	-1.12990899126695	-0.16372084837217	6.17814427083741
C	-0.56942447824899	0.69536613046695	5.22464402404443
N	2.07619959737040	2.04547303608972	6.60185599801074
N	0.18852835383167	3.97498454264356	6.68511779026272
C	3.05145178804458	1.10890713964974	6.51770498781250
C	3.36771068019754	0.30164113485954	7.65061124993967
C	2.71202367146173	0.48185559762509	8.85528100948460
C	1.71938309660408	1.49207834104500	8.97004116891294
C	1.43593971208955	2.25160637737298	7.79866541137873
C	0.44173193781678	3.28848519020076	7.84679510351514
C	-0.23578385011715	3.55793953504616	9.07056792520407
C	-1.20899175958725	4.59309282712402	9.05047998814537
C	-1.47478588952618	5.25783421244247	7.86687471232245
C	-0.77403262382564	4.92804933041768	6.66848373420795
C	1.01930145422577	1.78270615062797	10.18863753797470
C	0.07344890587216	2.78112799463160	10.23702945633211
C	-1.15080761663698	5.59522827826725	5.40329178017929
C	-1.46955898368408	6.97438044747305	5.39856494531717
C	-1.91167263219583	7.59698730470069	4.22504338388996
C	-2.06463346362066	6.84977126776233	3.04451843978382
C	-1.76112126673321	5.47816000817530	3.03995066633697
C	-1.29944237494698	4.85624545735555	4.20674245059033
C	3.83479848268013	0.95014611891963	5.27336985210829
C	4.21106461734904	-0.34165264581138	4.83407686885134
C	5.02380179825661	-0.49829544643278	3.70475450709237
C	5.49190000762655	0.63040398677283	3.01016151079652
C	5.13414711416165	1.91775469903428	3.44397606710709
C	4.30540924000236	2.07785401075277	4.56150635438634

H	3.01707091461897	8.06566806829471	3.79319759516995
H	2.97656094352236	7.48587747574066	1.36447539512104
H	1.25631253934963	1.03830559069860	-0.24079074830417
H	0.51781781017053	-0.42860953329030	1.64110299263163
H	2.63746884853915	5.69265375801396	-0.42545573640363
H	2.01109592391163	3.35617414969844	-1.00752744414964
H	1.58693262192177	8.44960542506461	5.62032097044712
H	1.92206207285682	9.13004531651071	7.98825400398505
H	2.99769762650651	7.55568356390305	9.60859074580055
H	3.73886361699032	5.29319224630478	8.84213864576671
H	3.42196452333220	4.61160832165324	6.47485540782304
H	1.35517199445953	-1.57563691495212	3.51982601138927
H	0.36771281351511	-3.09297476948362	5.22459326492656
H	-1.23855607645519	-2.19973806108442	6.92263238595661
H	-1.85387874042731	0.22456227042821	6.90120955251267
H	-0.88357782915579	1.74349157880308	5.19136672061379
H	4.17147289802100	-0.43273323037639	7.55911785065756
H	2.96877157074891	-0.13001928754230	9.72632209284663
H	-1.75958263148900	4.83990319983543	9.96422836086365
H	-2.25876916032353	6.01713509031702	7.81906375115555
H	1.25427102703129	1.19565826056563	11.08190941704228
H	-0.46134821671046	2.99564801153534	11.16750081795886
H	-1.34821532710407	7.56320032711459	6.31347667735515
H	-2.15045398885411	8.66483463498382	4.23396731517500
H	-2.43673510115503	7.33208909469249	2.13541637434235
H	-1.91139536812467	4.88687711812544	2.13137001755185
H	-1.11889249687680	3.77640622154227	4.20688016553102
H	3.84637225334949	-1.22487494329440	5.36825890441645
H	5.30431207283702	-1.50260494836068	3.37298120722495
H	6.14923818453333	0.50661168707200	2.14404355942003
H	5.52566137165714	2.79884601458471	2.92615360407305
H	4.07964751840856	3.08526030192473	4.92622000533860

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Bis-dpp triplet

Cu	1.37329558143494	3.30664451119019	5.20666024728706
N	1.92994983727168	4.86399047966279	4.09928684536791
N	1.26263211730809	2.33243842304847	3.47000283285024
C	2.33594930397769	6.11066693920210	4.46705136848115
C	2.71740789356818	7.06096119441951	3.48894220639864
C	2.71518254890074	6.73432873475825	2.13222591100788
C	2.35422225593333	5.42770493185158	1.73451351868383
C	1.97219238342673	4.51084711488043	2.76159985193847
C	1.60338098533541	3.17589826781821	2.42698306962611
C	1.60566296735873	2.75145023889734	1.06249662131440
C	1.22193153353265	1.41818882153807	0.79689845313880
C	0.83051413134867	0.59478457149146	1.85331935696146
C	0.84131506561087	1.06920065369411	3.18788108344855
C	2.35542724632307	4.97702554610052	0.36960411373504
C	1.98869222215781	3.69219548778789	0.04566174577714
C	2.43931784643776	6.47283393311249	5.90195883212495
C	2.03925422141642	7.75672289690048	6.34042104319059
C	2.21587563895958	8.14240892209073	7.67568855461500
C	2.80723955145181	7.25949430032267	8.59376971768864
C	3.21589227156862	5.98475440017089	8.16855190177944
C	3.02838919039187	5.59264917927707	6.83730294405118
C	0.33500645412102	0.18914341464174	4.26975785460172
C	0.66868770941536	-1.18514480744697	4.28158845702198
C	0.12656257987717	-2.04298402858394	5.24761242165847
C	-0.76822967068462	-1.54744761892694	6.20986713842412
C	-1.11364271899893	-0.18609088217375	6.20311560199672
C	-0.56335910405620	0.67530801800511	5.24584395862587
N	2.05645892557549	2.03549694944237	6.57546598909823
N	0.21034106785027	3.99076848987170	6.67240726873136
C	3.05177970210899	1.10911665459906	6.50290826982569
C	3.38993954614056	0.32630807994867	7.63350012885319
C	2.73314466584286	0.50476119661322	8.85184570496010
C	1.73730278305415	1.50054401545829	8.96318762579884
C	1.43265358034878	2.25797237511640	7.79071661046958
C	0.44356780426584	3.28214395678013	7.83788706459399

C -0.25440667754539 3.55002122313485 9.05547225042345
C -1.22974512375386 4.57174052883891 9.03272404751334
C -1.49133686199846 5.24214173084550 7.83711002944098
C -0.77247653614030 4.93221142438615 6.65668226408772
C 1.02743732663618 1.79154866259323 10.17867055965694
C 0.06472449905796 2.77227931550578 10.22132161989651
C -1.14321083921961 5.60701881210193 5.38849959853321
C -1.44575709500851 6.98857531626692 5.38252583165564
C -1.88374751317904 7.61860101595526 4.21035515027501
C -2.04109848520737 6.87846724161769 3.02733823063173
C -1.74992782546160 5.50442256045014 3.02237476254709
C -1.29886181695610 4.87551707439490 4.18954948270551
C 3.83307063995621 0.94544521810772 5.25247429572123
C 4.20284848585310 -0.34654054908841 4.81153162733426
C 5.01600771610642 -0.51010841817424 3.68243872039539
C 5.48581519683907 0.61257801289194 2.98172032580855
C 5.13087809268333 1.90099850985812 3.41385070437767
C 4.30740373781561 2.06628607276725 4.53446957581725
H 3.05084693182554 8.04613205558883 3.82323256268687
H 3.01412871428794 7.47170749638748 1.38026647481025
H 1.20988706453906 1.04832358815390 -0.23344339397594
H 0.47288998936685 -0.42007695337319 1.66445678763996
H 2.65323628651430 5.68337605093813 -0.41234577004856
H 1.98524513149945 3.36193389821383 -0.99836648911989
H 1.56701894557601 8.44411779203093 5.63125973000057
H 1.89326511815278 9.13723910107270 7.99939528111735
H 2.95642569468561 7.56629048717934 9.63387282015553
H 3.69630053934681 5.29806093914223 8.87271975159461
H 3.38188067839864 4.60987336014844 6.51031297401865
H 1.37602901596221 -1.57296396418037 3.54158674608257
H 0.40163222439388 -3.10265871402127 5.24699574934060
H -1.20067152902478 -2.22061497117304 6.95688444952405
H -1.82514424176641 0.20453731275422 6.93751925523284
H -0.86359668082641 1.72759245366330 5.23021623807049
H 4.20413684193960 -0.39636194219572 7.54193042636759
H 3.00033073713328 -0.10095832208408 9.72377693558130
H -1.78970836895768 4.81276948722029 9.94206686664399
H -2.28274144098169 5.99313651678099 7.78209180150125
H 1.26817719163238 1.21031246836164 11.07490422076059
H -0.47597253942801 2.97966450925306 11.15066636404772
H -1.31283318586364 7.57176117210023 6.29950293512933
H -2.10633356057695 8.69046157314983 4.22183127317929
H -2.39605797420224 7.36846719966273 2.11515000331391
H -1.88840198230742 4.91661104614629 2.10941584752448
H -1.10416999593823 3.79843918145394 4.18098785422582
H 3.82908461086751 -1.22487802943315 5.34756714909521
H 5.28667296809489 -1.51777643363166 3.35092052124268
H 6.13175020104537 0.48448349076499 2.10732906470345
H 5.50868788736157 2.78168246488620 2.88482833815286
H 4.06174968819671 3.07582657102484 4.87893365845266

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97

Bis-dpdmp reduced

Cu 1.36614462690101 3.30470758490210 5.20405765322100
N 2.05615457478802 4.83203517190393 4.07826855453536
N 1.13929927804906 2.38497110262452 3.42077408145520
C 2.43997228371513 6.08207792571537 4.43054272152974
C 2.79393973620050 7.04719662589197 3.45070385332359
C 2.78005443488103 6.75758968224926 2.09124074756628
C 2.37262928956582 5.44061678850495 1.70820911169788
C 2.00410397848834 4.52440638224735 2.73954406223918
C 1.55550710203238 3.19280129199990 2.38949499121714
C 1.55952346962423 2.78170576486820 1.02195797859268
C 1.14633835769052 1.44580666332425 0.71904232078609
C 0.76112619720757 0.64350097452499 1.78671762273312
C 0.75312541368253 1.12113569415651 3.12415485474395
C 2.33661248553342 5.00212902805818 0.34357235118789
C 1.95952372204899 3.72088092036300 0.01515903272797
C 2.53697817378442 6.44852947141538 5.86655419150734
C 2.20130708231392 7.75698799238218 6.28596829734066

C	2.34912232304761	8.13938585624807	7.62548289088787
C	2.84834224978730	7.22636838670237	8.56830011350040
C	3.18356410151422	5.92411398863939	8.16385398744168
C	3.01960780606095	5.53501628484288	6.82828276133727
C	0.27010101459456	0.22183013869839	4.20316591994730
C	0.55621803551924	-1.16238167362382	4.15072596237603
C	0.05244462997539	-2.03468206431079	5.12419305758070
C	-0.75838831667145	-1.54303733685583	6.15990429577102
C	-1.04794599532896	-0.17049673386759	6.22310369230780
C	-0.53010299459816	0.70537304349628	5.26041941523865
N	2.13882980467412	2.11532046811990	6.64267807174369
N	0.11453232268193	3.89223347980980	6.67338379213031
C	3.10744035164056	1.17087789766567	6.57972662899239
C	3.43399427088784	0.37494640913391	7.70991224465470
C	2.79269848655770	0.53176406454032	8.93308721364955
C	1.76442512408079	1.52380901768632	9.00890788555034
C	1.46572375472645	2.27314404192628	7.83075677066082
C	0.40845699594975	3.26220054441352	7.85907078633318
C	-0.27333920523476	3.53509214945742	9.08362816844897
C	-1.28589528473948	4.54607837550244	9.07999956259735
C	-1.53882199134288	5.18642423140856	7.87229199128136
C	-0.84441580298474	4.84823092804386	6.68079500892185
C	1.04036756042941	1.80563459594284	10.21393825945846
C	0.07156451735777	2.78113916384235	10.25338762810175
C	-1.21241388777636	5.53376260188037	5.41572377128377
C	-1.55315258993751	6.90622923447027	5.42953851079738
C	-1.96331733324089	7.55338309564815	4.25669442790868
C	-2.05479136397600	6.83784797219828	3.05201591268680
C	-1.71916767499272	5.47451289245766	3.02648911019466
C	-1.29181433653507	4.83023616231563	4.19461096370060
C	3.87853570889253	0.98389056219895	5.32409003715824
C	4.30701403166018	-0.30927819803373	4.94342731527100
C	5.09128532502070	-0.49506209630514	3.79769849471867
C	5.47430820575438	0.6086662893446	3.01869054353107
C	5.05303279443029	1.89697974355007	3.38543106279416
C	4.25401206912992	2.08202759955339	4.52088225732841
H	3.13854456309299	8.02869269635070	3.78805205383490
C	3.19720737765409	7.78732880256715	1.07117385944919
C	1.11065395297815	0.92738813567454	-0.69696395350842
H	0.40059723095346	-0.37090460482614	1.59453409736011
H	2.62457780313651	5.70132802324131	-0.44630478624028
H	1.95523065470793	3.40953127273028	-1.03304420439133
H	1.79663297708287	8.47083605938182	5.56116778304761
H	2.07622019281340	9.15413211646627	7.93285495727450
H	2.97909155576747	7.52980626106989	9.61207909980841
C	3.58437759411592	5.20971176435682	8.89016765740028
H	3.29039171960801	4.52211197326559	6.51967199679311
H	1.20067187705366	-1.55234269967007	3.35622659321909
H	0.29172686869684	-3.10177082459774	5.07191861499459
H	-1.16548471873793	-2.22703894326188	6.91160723936927
H	-1.68846829705559	0.21944331816287	7.02074952094404
H	-0.76365192229371	1.77174746226030	5.31244404445510
H	4.25332369940652	-0.34377492504757	7.62073239042214
C	3.18389791375455	-0.29902752350570	10.12966620773677
C	-2.06325970075290	4.89549880861773	10.32443730725906
H	-2.33203354560863	5.93728862831607	7.81656039178311
H	1.27367833898605	1.23718504693446	11.11845613242518
H	-0.45477923554213	2.98427996075420	11.19009006658083
H	-1.46991347719298	7.47485635329030	6.36146927726245
H	-2.21496974575732	8.61854573752876	4.28466092155293
H	-2.39064402468220	7.33935470974996	2.13859133127467
H	-1.80065299232397	4.90667258282901	2.09402572283615
H	-1.04326217741708	3.76620483025198	4.16908509656153
H	3.99984770066684	-1.17777190469474	5.53498551778336
H	5.40617293343010	-1.50460754517760	3.51427293202422
H	6.10074002592321	0.46545577874991	2.13227943795409
H	5.35592290974883	2.76418979789511	2.78983116134296
H	3.93254393675274	3.08790127820865	4.80255688641018
H	2.11071720091249	0.96389317002555	-1.16603885547863
H	0.43317361974234	1.52670552525585	-1.33205433919199

H	0.76257080340305	-0.11704004132134	-0.72594943930197
H	4.05992844267116	7.44069933661338	0.47361403130179
H	3.48354378601351	8.73247653051292	1.55853921918493
H	2.37948911725713	8.00739661594664	0.36088027169649
H	3.98933543116461	-1.00520639450790	9.87386248123267
H	2.32873335901404	-0.88547319349406	10.51204139071787
H	3.54129352305638	0.33294278501701	10.96304351275992
H	-2.79562310879250	5.69263420915581	10.12175594170073
H	-1.39629993900767	5.24662665362846	11.13275124118206
H	-2.61524913792181	4.02208185383245	10.71689824648420

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Bis-dpdmp oxidized

Cu	1.36365032920625	3.30490041251968	5.20369112333762
N	1.94608476977415	4.85518544831271	4.07768126623118
N	1.25202885215695	2.34168848052992	3.45071951206214
C	2.32113829613584	6.10219063520216	4.44622056943882
C	2.67839736220516	7.06421731144682	3.46168528092659
C	2.68784338093574	6.77088935297939	2.10299809192969
C	2.33614305427842	5.43328702664066	1.71823500318415
C	1.97209203883515	4.51761094617600	2.74613736867867
C	1.61412687122349	3.16315030898161	2.41097564225022
C	1.64067180229517	2.73387527453461	1.05347051130575
C	1.27453844047458	1.37491201685051	0.77059870773367
C	0.88591052988737	0.58475517348733	1.84615819335781
C	0.86124264198610	1.07436676994366	3.18097340460293
C	2.34936866490601	4.97400734855819	0.36044157892480
C	2.01447741163044	3.67701167858331	0.04090017805711
C	2.42179483235665	6.46574811627432	5.87799951232619
C	2.01937923704449	7.75073173673074	6.31271816122874
C	2.19532092640632	8.13727024730724	7.64708733600388
C	2.79406409345606	7.25634525296718	8.56363422445277
C	3.20604317276999	5.98180674062987	8.14123098473321
C	3.01525204031539	5.58563890547977	6.81135238627375
C	0.34721409943602	0.20005351465961	4.25970479674833
C	0.68078447736078	-1.17479811436881	4.27805224138627
C	0.12766325239077	-2.02733610238271	5.24155028756944
C	-0.78244223356384	-1.52636975341262	6.18776809491546
C	-1.12909335825239	-0.16541230095767	6.17222069851295
C	-0.56401720397919	0.69347152209558	5.22092521318950
N	2.06800032165787	2.05230638752578	6.59903277484285
N	0.19037801259215	3.96447813861271	6.68632333806456
C	3.04708785357552	1.12217259594435	6.51409793783382
C	3.37021973419810	0.31561135996327	7.63977942538977
C	2.73194084020957	0.45968720856521	8.86634414977731
C	1.72805863988277	1.48088725126618	8.96757249060829
C	1.43477743455909	2.24551487087527	7.80266111363587
C	0.43722710944405	3.28334302021037	7.85359458175296
C	-0.24337748327172	3.55834750715504	9.07371787682290
C	-1.22884587413299	4.60215455056577	9.07331155624071
C	-1.47046543302134	5.24723743904477	7.86585163159913
C	-0.77084083549394	4.91691743090326	6.67267696049038
C	1.02334737752203	1.77707479566167	10.18011911482469
C	0.07571923847110	2.77508470722730	10.23100659464335
C	-1.14800712671528	5.58683280317929	5.40727485718369
C	-1.44766062342989	6.96958071784081	5.39947734963014
C	-1.89226996153437	7.59366029726490	4.22734622721905
C	-2.06487614368448	6.84449930694685	3.05110152893510
C	-1.78012277660939	5.46917099728829	3.04991794969947
C	-1.31821368501915	4.84541895748024	4.21593608136911
C	3.83377804824795	0.97099524631396	5.26892285611448
C	4.20717316119989	-0.31710878646838	4.81837622852265
C	5.02542940213235	-0.46621027272084	3.69175719488743
C	5.50082507070938	0.66695138914345	3.01014925099653
C	5.14543997499880	1.95082180153183	3.45512859859935
C	4.31268861446317	2.10311424149401	4.57111581805329
H	2.99568457600924	8.05271906240441	3.80446315181110
C	3.08218595647221	7.80746675144885	1.08520590369402
C	1.27900710856537	0.83158139299734	-0.63323088058588
H	0.54318459126646	-0.43851062838706	1.67048163524163

H	2.63487663556658	5.66983045836653	-0.43268339803083
H	2.02983001898934	3.35634486669367	-1.00391836719223
H	1.54777656324396	8.43950716248474	5.60455321602349
H	1.87623113467463	9.13293427637215	7.97020834391692
H	2.95490612425306	7.56966782024296	9.59980826155673
H	3.70153069110157	5.30486017264864	8.84413450258476
H	3.38927413749527	4.61145281036861	6.48061861653090
H	1.39277953947025	-1.56971846759815	3.54632071682887
H	0.39716825998644	-3.08796306062508	5.24656857262555
H	-1.23372712047846	-2.19918252804165	6.92354460001037
H	-1.86207620488599	0.22177435847788	6.88683269151932
H	-0.88262686266502	1.74004309178851	5.18201371356915
H	4.18127691365469	-0.40972144184348	7.53280742737094
C	3.10521357568617	-0.40062994758488	10.04381220080115
C	-1.99396256518037	4.96683392078911	10.31733518280907
H	-2.25309926944761	6.00831186587670	7.80561898563192
H	1.24874218103568	1.19910732744121	11.08006108563019
H	-0.44808472223649	2.97590497889894	11.16910816515221
H	-1.31003898073771	7.55911477547317	6.31152843386521
H	-2.11708841264715	8.66464053174397	4.23448430661574
H	-2.43746436679237	7.32847126757321	2.14299954982386
H	-1.94389565375327	4.87612627768110	2.14475438607329
H	-1.15217441955746	3.76333744649445	4.21889926889987
H	3.83589917263180	-1.20341514034212	5.34279066976349
H	5.30376970754578	-1.46855280557058	3.35199805083930
H	6.16139178046401	0.54917522795141	2.14557846257341
H	5.54002905232435	2.83615721583133	2.94684410483159
H	4.08856064361495	3.10806198049189	4.94315977991768
H	3.88695538622376	-1.12731903622205	9.77565546641397
H	2.23222352801901	-0.96260217134873	10.42197048928331
H	3.48454871892087	0.21036631046944	10.88304739905322
H	-2.70116431799157	5.78781618622937	10.12507904825278
H	-1.31294251076683	5.28568747969921	11.12696872779939
H	-2.57113266059529	4.10586470614263	10.70084557345656
H	2.28297376254323	0.90716352330923	-1.08842373191760
H	0.58591287868480	1.39546823573349	-1.28377149575011
H	0.97493999766289	-0.22585915749464	-0.65316583273532
H	2.27273410163587	7.97777626893927	0.35261232403326
H	3.97351436232662	7.49004257187969	0.51395425001148
H	3.31470829504367	8.77019214953085	1.56493258429774

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Bis-dpdmp triplet

Cu	1.36594190001085	3.30492745941406	5.20354915179321
N	1.91744853352965	4.85707034510222	4.09330721702224
N	1.27561377113228	2.33619449753773	3.47127730837279
C	2.31158504109429	6.10589021559470	4.45966399442219
C	2.68511611684255	7.05875611055379	3.48544387499284
C	2.69726477838059	6.76453205616583	2.11588715339913
C	2.34482711706957	5.43833566816433	1.73085593845838
C	1.96832013791396	4.51316726682759	2.75275208840876
C	1.61338747800286	3.17155006836605	2.41948851639015
C	1.62292425935208	2.73615034999773	1.05843973334995
C	1.25316922139078	1.38885642334499	0.77699253713449
C	0.86699850723520	0.59052910314375	1.86131483544929
C	0.86709379328982	1.07002466815303	3.19058970751276
C	2.35176005832109	4.97601540679784	0.37181303062635
C	2.00025809896003	3.68495810726799	0.04944954533656
C	2.41422325290824	6.46964304166804	5.89489185713429
C	1.99755253875518	7.74683996368685	6.33642104715396
C	2.17747048592324	8.13556559374739	7.67041407899033
C	2.78839373592418	7.26196982084640	8.58443395101373
C	3.21216298887922	5.99312185592301	8.15633637634081
C	3.02172232143056	5.59816980099761	6.82634477995195
C	0.35626368541644	0.18898316392856	4.27035606367927
C	0.69713814473633	-1.18335152658978	4.28913503540563
C	0.14514109462464	-2.04381595284074	5.24720767570052
C	-0.76692090796925	-1.55304065696098	6.19540414020394
C	-1.11792182910875	-0.19310693335757	6.18319200401588
C	-0.55756508891462	0.67087310369339	5.23413692713963

N	2.05009075728968	2.04163695143139	6.57526876190672
N	0.21614998016572	3.98606485414626	6.67320146336755
C	3.04339022083322	1.11575907575400	6.50254959250626
C	3.38155974838390	0.33152486237474	7.62842989611281
C	2.74237368326454	0.48204213303965	8.86569934328265
C	1.74267843067484	1.49291506923503	8.96421904189834
C	1.43239591374066	2.25564904464257	7.79629718023826
C	0.44419358999277	3.28432572265400	7.84515781339445
C	-0.25386277680324	3.56152646684235	9.06083030408126
C	-1.23675485164005	4.59353227787211	9.05587938398289
C	-1.47661021675126	5.24400452460714	7.83872657758482
C	-0.76353369870869	4.92916070865122	6.66006102362117
C	1.03163322397399	1.79322965758704	10.17454965675616
C	0.07185137299986	2.77865158872420	10.21914238597436
C	-1.14235159493667	5.60180204029758	5.39232069201779
C	-1.44050367826548	6.98420121302762	5.38283237376716
C	-1.89091712619837	7.61032997308801	4.21319849787041
C	-2.06449621845509	6.86572508324038	3.03541498063846
C	-1.77730147301703	5.49083920392233	3.03373296819383
C	-1.31501002856768	4.86596777944212	4.19860668889527
C	3.83109393166446	0.95460624047735	5.25485706446789
C	4.20146053089682	-0.33587106094803	4.81035790096861
C	5.02435332620939	-0.49647817182808	3.68786286150566
C	5.50315195300009	0.62802402974552	2.99649557553797
C	5.14689046111766	1.91507308598529	3.43157457965940
C	4.31432247022276	2.07713543378740	4.54591157393808
H	3.00902135221618	8.04468704799411	3.82993682012956
C	3.09893814828823	7.80784328168161	1.10358679814678
C	1.24337595375204	0.84234202970849	-0.62863686561573
H	0.51543073986998	-0.42956515202026	1.68403889489801
H	2.64148703865037	5.67110173511250	-0.42130263428369
H	2.00908929473419	3.36790789357958	-0.99722174050047
H	1.51025655678036	8.42627735985986	5.62975582370363
H	1.84233512147536	9.12565453823126	7.99627849477046
H	2.94045021304537	7.57109947435721	9.62350722357752
H	3.70645498488600	5.31315438398055	8.85750599631325
H	3.38300761530052	4.61887176178140	6.49708596156369
H	1.41697875650697	-1.56742831460497	3.55924372486231
H	0.42592243187345	-3.10208112469724	5.25105584144651
H	-1.20784032431590	-2.22834950568079	6.93561208186739
H	-1.84230479119495	0.19418853995746	6.90678820106065
H	-0.86152532865219	1.72212678068580	5.21578067473100
H	4.19792816676899	-0.38856282249061	7.52543469101459
C	3.12741796929780	-0.37539729788825	10.04516269080229
C	-2.01527127288053	4.95831878680919	10.29500002019112
H	-2.26582312905803	5.99808901818882	7.77465787459104
H	1.26059730221949	1.22078173952280	11.07787843276445
H	-0.45646983291263	2.97630528725549	11.15613037168382
H	-1.29526423273125	7.57072625234687	6.29569503190342
H	-2.11013190954061	8.68300325651832	4.22266945983802
H	-2.42869178365626	7.35274705296147	2.12517896275325
H	-1.92755656047986	4.89908734368590	2.12511995491828
H	-1.12216803023581	3.78864104977555	4.19260963648658
H	3.82034003584935	-1.21536876329113	5.33918541335590
H	5.29514475772196	-1.50344353489192	3.35400475881652
H	6.15658470560353	0.50243686681459	2.12723636756880
H	5.53063677086836	2.79749501441685	2.90966262737325
H	4.06725922933826	3.08551113851336	4.89239792038406
H	3.91758767527934	-1.09207389755965	9.77121675991207
H	2.26514618611961	-0.95340843026529	10.42505831877271
H	3.50412101916574	0.23378405783407	10.88739555682990
H	-2.72934999186465	5.77083134780852	10.08776853197927
H	-1.34747335415369	5.29590229120829	11.10866846338249
H	-2.58963196508122	4.09777834697355	10.68473665791501
H	2.24577219250396	0.89570276020854	-1.09158150532154
H	0.55516648462910	1.40908898784711	-1.28246175179719
H	0.92381923379236	-0.21159342601032	-0.64037402955316
H	2.28972369754399	7.99871621310758	0.37509243803270
H	3.98729353102434	7.49468713470228	0.52471868290390
H	3.34009817543464	8.76327668699834	1.59553561426015

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Bis-dptmp reduced

Cu	1.36589482820448	3.30549922900268	5.20317521383858
N	2.12881509018510	4.79665944722883	4.08910412771356
N	1.06931777758141	2.41185863512394	3.42722328997234
C	2.64526470475873	5.99312547223018	4.45636389481509
C	3.20638640040270	6.91302928340909	3.51184915232666
C	3.13195941574475	6.60946824792273	2.13944527638041
C	2.54901057503465	5.36728180158687	1.74331548333903
C	2.07749293393791	4.48646646098573	2.75686911539338
C	1.50536345271110	3.20600014725601	2.40091050360100
C	1.42394642136670	2.81272721044618	1.03566166374237
C	0.82890536909224	1.55185659020300	0.72582197011341
C	0.35596167561165	0.75090654428677	1.78224139003258
C	0.54203811935657	1.20065540190546	3.13003953874195
C	2.44556752358006	4.94416978646877	0.37336526509706
C	1.91417136498771	3.72221920370768	0.03601222071342
C	2.59320526534296	6.32020319950403	5.91344315413588
C	1.97547851936296	7.51295681581438	6.35064708807561
C	1.92138447824794	7.83367010791246	7.71451414706810
C	2.49539666697884	6.97299637576925	8.66376909214923
C	3.11532801734053	5.78709006082902	8.24027619903666
C	3.15424028550068	5.45804273912624	6.87754045468744
C	0.16831777300184	0.33612444259993	4.29000100057139
C	0.69354388863074	-0.97080307231247	4.39765890023134
C	0.35138341081115	-1.79392872641698	5.47994360373263
C	-0.53187881939468	-1.32860863780555	6.46711688353492
C	-1.06271926746249	-0.03303628220099	6.36844496126251
C	-0.70696844143056	0.79639778894927	5.29502312048132
N	2.19914980435679	2.19172431485726	6.65732950036018
N	0.06360015999346	3.82982667891741	6.64519033553098
C	3.26866110761765	1.36207808299473	6.62375668188133
C	3.75198590414058	0.68050705243205	7.78763122656446
C	3.03458084751303	0.79847445069077	8.99300691132883
C	1.88232516461091	1.64170703648199	9.02452953558389
C	1.51383166424514	2.32946308246736	7.83426679373675
C	0.36651372251402	3.21114344890346	7.82803353459608
C	-0.38901464538676	3.41241555427567	9.01731078942721
C	-1.52832274913640	4.27168237610115	8.96138306362172
C	-1.85207111535290	4.88464119361994	7.73623864658019
C	-0.99628164019729	4.67173477608415	6.60714687076155
C	1.09421545104005	1.85998773714110	10.20694836337011
C	0.01448045123765	2.71050490868198	10.20532906693286
C	-1.23120827727755	5.38576273249193	5.31575602951059
C	-1.30918394724819	6.79585104219828	5.28788268001607
C	-1.53243931555419	7.47756930042430	4.08312945242505
C	-1.69404658933323	6.75992796724537	2.88723015343033
C	-1.62251522030611	5.35825405247228	2.90380155569550
C	-1.38227279303433	4.67746009195287	4.10611882512799
C	3.92627161598511	1.18107184666963	5.29440350834981
C	4.09539179720892	-0.11375387795443	4.75580955414198
C	4.71264257549449	-0.29674150783361	3.51020222296010
C	5.18263547278760	0.81127308031693	2.78732763685204
C	5.02324580067184	2.10228525578753	3.31453261010988
C	4.39060384707604	2.28653595358967	4.55249494251079
C	3.92898831129838	8.16271494705531	3.97913192680571
C	3.66447763697820	7.55303187255553	1.08464428309391
C	0.70969033843176	1.11823755751853	-0.71797678093073
C	-0.39542815064089	-0.53405092952802	1.48804409503895
H	2.80697491689104	5.60545920148983	-0.41842820407397
H	1.85316112704041	3.43988503116003	-1.01820984236242
H	1.52408708533062	8.18355501185527	5.61260609745599
H	1.43662526755908	8.76180094717633	8.03524737568142
H	2.46691650415599	7.22982599961574	9.72769789836765
H	3.57788682376023	5.11726644652812	8.97229764202988
H	3.65868571272945	4.54272333728562	6.55839537967301
H	1.38587810182398	-1.33444539876871	3.63179382902474
H	0.77004468087790	-2.80358358221934	5.54770061411243
H	-0.81156198823997	-1.97599957139345	7.30459868692129

H	-1.76332827947879	0.33257540306102	7.12604222389348
H	-1.14395136919964	1.79506255450723	5.21852464293374
C	5.05104323649519	-0.10244937228823	7.74684432476884
C	3.46274232795155	0.07122062868052	10.24770292741450
C	-2.36293802678729	4.48802982370138	10.20370329839145
C	-3.12418077151790	5.70108825585273	7.60529382475658
H	1.36642995595846	1.34571988863317	11.13230865538209
H	-0.55787206503063	2.84746447050577	11.12647668633894
H	-1.17938040664578	7.35739846846534	6.21841854617695
H	-1.58772878200251	8.57128169106586	4.08039009694296
H	-1.88337531951391	7.29055865061671	1.94844644983693
H	-1.76174638703494	4.79019096529804	1.97837299889016
H	-1.35049516398824	3.58513826746854	4.11001941274420
H	3.72596684147788	-0.97891340332491	5.31544104757165
H	4.83328217165674	-1.30793857628553	3.10746314366770
H	5.67819850833021	0.66816759995121	1.82158824192525
H	5.39943824734186	2.97066731428383	2.76421130735183
H	4.29167358620106	3.29479032532989	4.96221213508999
H	1.67072682928394	1.23853417169730	-1.24774215054299
H	-0.03660051946429	1.72680515078211	-1.26281357579653
H	0.41325739536178	0.06493999203828	-0.81473450078905
H	2.92070227756565	7.71414860302589	0.28480049084729
H	4.57336340852338	7.14714876072807	0.60168357593663
H	3.91968661589997	8.53894648406521	1.49618787949985
H	4.22508569262448	-0.69373195996037	10.04667150107647
H	2.60618728336689	-0.43678195563609	10.72375084463889
H	3.88042848274190	0.76956486427713	10.99749692169956
H	-3.07508991706123	5.31645179063230	10.08819871851739
H	-1.72574817466967	4.72190941487403	11.07410541869710
H	-2.94351838169872	3.58257416608997	10.46333964032917
H	5.62356677219541	0.10911293616690	6.83338471398647
H	4.88166211647924	-1.19470903190266	7.78437417735948
H	5.68989960659247	0.15480257978133	8.60898909090276
H	-3.37850072021588	5.89098079831460	6.55353061302369
H	-3.04266379059817	6.68332663117224	8.10703972148083
H	-3.97699831134152	5.17337369249309	8.06552570924656
H	-1.14245370851838	-0.37634594602799	0.69145729212338
H	-0.92734385900400	-0.90536273951942	2.37475668824924
H	0.27752025873495	-1.34195009261960	1.14519356689937
H	4.89670727966947	8.27210533514934	3.46031936656680
H	4.13154570623280	8.13474658988403	5.05852298930356
H	3.34746646193804	9.08130103409860	3.77655113963479

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Bis-dptmp oxidized

Cu	1.37287946521022	3.30370201708562	5.20171018988801
N	2.01620974440379	4.83916012457932	4.08874931789789
N	1.18608890719860	2.36482906423115	3.43753622304322
C	2.51124495078388	6.03542300886686	4.48393059404767
C	3.03631614603231	6.97823357261892	3.53813924520425
C	2.94934997383149	6.69121612029116	2.16229426474461
C	2.44702128558936	5.41433766320763	1.75438599365149
C	2.01742498442362	4.50915756175878	2.76190487559685
C	1.55614042701766	3.18880919935071	2.41140107269882
C	1.50294427924602	2.78138664083282	1.05050401589345
C	0.98647831759004	1.47904833615012	0.75630211759716
C	0.51646810403728	0.67968512850927	1.81637614890023
C	0.67505119086867	1.14111373645233	3.16548437232976
C	2.38935281060750	4.97434279018618	0.38737684853258
C	1.93407317787895	3.72084093920755	0.05145507764656
C	2.51146555059603	6.32731548050003	5.94609242751545
C	1.90521865692103	7.50203866609627	6.44542423189710
C	1.93944538703411	7.79459798061642	7.81532388342586
C	2.59720977154373	6.92925141420247	8.70599356527807
C	3.21495689838871	5.76711565453887	8.21949376333076
C	3.16560009534832	5.46325702112437	6.85096041891626
C	0.25975806275114	0.29926605054312	4.32358787293404
C	0.75510620604924	-1.01581710497504	4.47258493201813
C	0.33301726049961	-1.81968750525089	5.53987514220424
C	-0.60547180732537	-1.33046368936762	6.46433994012931

C	-1.11360035032755	-0.03056111554762	6.31921050452004
C	-0.67817000240904	0.78189187590770	5.26198920532089
N	2.11954939645791	2.09803571070427	6.61865648585407
N	0.14122932396533	3.92434066385331	6.66137962743432
C	3.18137625262453	1.26055043037306	6.56202534260900
C	3.65409916682522	0.56711794287103	7.72740842349886
C	2.93689202175669	0.68606998460384	8.93292740787972
C	1.82617034078687	1.58746468802421	8.98875309852083
C	1.47511235898837	2.29531816170722	7.80837516547958
C	0.40276352229890	3.25818096132409	7.82623904492833
C	-0.33464633542355	3.49256068228182	9.01759896904091
C	-1.42731017298018	4.41583064669209	8.96656394831730
C	-1.74943700267027	5.01851265992419	7.73557078789352
C	-0.90386534791011	4.78231346347519	6.59945013060034
C	1.07008418631181	1.84992856121510	10.18247046747701
C	0.03496772453346	2.75578732079180	10.19500285195771
C	-1.15823219527855	5.45819436753835	5.29497652410334
C	-1.24691027192940	6.86652642251068	5.21939626369879
C	-1.52441196045585	7.49897477054006	4.00020437356134
C	-1.73768247021792	6.73430350750761	2.84066327330208
C	-1.66499480579842	5.33454845842421	2.90654925650609
C	-1.36906888037079	4.70079576519889	4.12242444883835
C	3.85776572263708	1.10290535156669	5.24306133514870
C	4.05696388881438	-0.18011524902567	4.68505957662906
C	4.72594626758780	-0.32978920046853	3.46300537919753
C	5.22387322767866	0.79753884764550	2.78773122035291
C	5.04204617092744	2.07548877249529	3.33795884380692
C	4.35639629551134	2.22850689542938	4.55197523570173
C	3.71943044902465	8.24813080386851	4.00231568916176
C	3.41694744358479	7.69025684861668	1.13237742716652
C	0.90353386568029	0.98699276867950	-0.66777849125964
C	-0.18680713647719	-0.62730287753998	1.51445608372407
H	2.72483194573601	5.64606089472624	-0.40600901232527
H	1.89092324094792	3.43959987334558	-1.00305048884652
H	1.40369102789787	8.18480731157250	5.75318342775377
H	1.46778950438553	8.70989880986780	8.18674592869912
H	2.64514672954019	7.17232679621196	9.77201170508809
H	3.75609722667053	5.10563945307777	8.90323429157200
H	3.69657620966486	4.58268173898012	6.47713554379229
H	1.47765851903822	-1.40372573587814	3.74852715235583
H	0.72351812126911	-2.83734285076133	5.64029731504664
H	-0.95339739371661	-1.96870432800753	7.28250535121600
H	-1.86751171125561	0.34535491669527	7.01793667665569
H	-1.11958921829673	1.77425985264693	5.13043264317844
C	4.93340407787410	-0.24405971175062	7.68268580758358
C	3.33991753235250	-0.08492469543468	10.16621162598979
C	-2.23446265713022	4.69580972720083	10.21068490452561
C	-3.00040555009633	5.86446334261731	7.61096959124849
H	1.32804269192900	1.32437093238239	11.10483200684114
H	-0.52469044529174	2.91075265924215	11.12033870081251
H	-1.09464215247763	7.46416145704911	6.12299854692176
H	-1.59296306566786	8.59064648766599	3.95838026724934
H	-1.97962634044630	7.22847823567030	1.89459961090046
H	-1.86034193393916	4.73204107445737	2.01395431924417
H	-1.36502659921957	3.60779569690949	4.17130259994982
H	3.68016236740386	-1.06098233078544	5.21324409023410
H	4.87540784048156	-1.33043835173073	3.04518264385853
H	5.76862595469589	0.67662551200699	1.84624316381029
H	5.45365219371525	2.95451693721009	2.83224488537222
H	4.26481297620346	3.22451623673354	4.99532189133804
H	3.99430294013227	-0.93475766923811	9.92977423174582
H	2.45807913841879	-0.48376411540775	10.69428897251708
H	3.88147223727592	0.56251581172968	10.88220658887905
H	-2.81597698291159	5.62412210177475	10.12736604157140
H	-1.58617427428889	4.79050488404456	11.09710226602804
H	-2.94819613026313	3.87501948223213	10.41614554422598
H	1.70572724017827	1.40139167186210	-1.29678756682423
H	-0.05999994686987	1.27413598686445	-1.13170693736349
H	0.97429869390778	-0.10944656683153	-0.72286702845777
H	2.79880957823117	7.65722930737034	0.22157462228199

H	4.46142564908406	7.48711218723120	0.82635926602329
H	3.38391558936628	8.71998753530275	1.51586710771500
H	5.53664868515517	-0.00844919089776	6.79554473527627
H	4.73552665658412	-1.33189771669824	7.66891050097024
H	5.55271383550945	-0.04022644747963	8.57179324034647
H	-3.28766673332164	6.01972933239584	6.56227911645542
H	-2.87427267998429	6.86224854655381	8.07069250268809
H	-3.84841368298406	5.37918030661915	8.12203564100759
H	-0.88607204242046	-0.50382298665089	0.67069104631401
H	-0.76134589157918	-0.99441036977456	2.37564450989774
H	0.52500941140042	-1.42361015212056	1.22706625388013
H	4.64404851870262	8.42302160496978	3.42757980996336
H	3.99002342902486	8.20288015457043	5.06594096901041
H	3.07920512911113	9.13889759711195	3.86144893952350

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Bis-dptmp triplet

Cu	1.37002090172586	3.30253940102017	5.20395022016748
N	1.98084890506636	4.83958447574482	4.10440861045469
N	1.21340895349871	2.35487452199176	3.46209515541058
C	2.49198399463884	6.03790674440644	4.50070914448570
C	3.02215566679719	6.97012122080481	3.56576297800237
C	2.95461404359733	6.68089794650314	2.17733542394999
C	2.46081469936197	5.41195500142329	1.76627140749344
C	2.01342172346627	4.50059220706259	2.76869249195097
C	1.56021340670018	3.19059698272348	2.42219741656218
C	1.49215531367043	2.77355570941704	1.05910934366663
C	0.97692500207171	1.47902795730712	0.77319041319383
C	0.51584366488132	0.67467287332577	1.84830315708488
C	0.68403357804008	1.13183615335470	3.18553838775534
C	2.40205289988849	4.96259158376464	0.39997882159956
C	1.93146287600295	3.71600427001100	0.06377028940253
C	2.49415160050065	6.32589028651272	5.96638510281046
C	1.88602287963185	7.49456798926776	6.47596646519101
C	1.92206611118473	7.78182249496557	7.84781154967818
C	2.57722133457056	6.91237196634424	8.73434329168207
C	3.19587357896445	5.75360879819006	8.23932541377070
C	3.14968816126492	5.46098252099788	6.86895389083650
C	0.26217351663793	0.29375927296007	4.34768454356143
C	0.75591046672577	-1.01954455846000	4.51127067145369
C	0.32909415341587	-1.81767116837731	5.58200646370904
C	-0.60865449788122	-1.32227331245652	6.50210655619880
C	-1.11558401805364	-0.02286337311267	6.34447597605588
C	-0.67950200984664	0.77903576002286	5.28023591794981
N	2.09623699119906	2.08323439101388	6.59366168952598
N	0.16935238079115	3.94299290616587	6.65281166805001
C	3.17447683854662	1.25385317656256	6.53965188217716
C	3.64979364831194	0.56912032996014	7.69322170392885
C	2.94133414152817	0.69006698836059	8.91747328772664
C	1.83943777945803	1.58679635057524	8.98443945384902
C	1.46962924591463	2.29661045394876	7.80303933749333
C	0.41028862827447	3.25502126195116	7.82264885713443
C	-0.34345887879982	3.49240712221109	9.01054644875692
C	-1.42398923987448	4.41551301256316	8.95289211539448
C	-1.73369226724395	5.02724934000892	7.70979739678883
C	-0.89087073669529	4.79468474107620	6.58709468841185
C	1.07742379133676	1.85604801157360	10.17555139338844
C	0.03450311701534	2.75089568949660	10.18495368407121
C	-1.14853285626477	5.46162192302127	5.27573969644872
C	-1.23646584091199	6.86845685973325	5.18322676585228
C	-1.51600779092469	7.49060911784410	3.95832086576637
C	-1.72489208796923	6.71733712718241	2.80519601556521
C	-1.65137013882502	5.31786491836394	2.88577498235769
C	-1.36051514003493	4.69681040028459	4.10865178522350
C	3.85606911697859	1.10823416798173	5.21878613356795
C	4.06024874043173	-0.16657398293174	4.64535343372947
C	4.73377790779825	-0.30365672572529	3.42341084899297
C	5.22629251253959	0.83010338223975	2.75751511004060
C	5.03878085507790	2.10177594626458	3.32135390654118
C	4.35485233732360	2.23919463593323	4.53755826774472

C	3.69187524211354	8.25109508774602	4.02003949606264
C	3.44338448313428	7.69964466263498	1.17442148140889
C	0.87235324380100	0.96550050651949	-0.64381114269481
C	-0.17826811145269	-0.63682733806002	1.54156008142848
H	2.74517642440708	5.62698970514887	-0.39689399469753
H	1.88774871487082	3.43885950041056	-0.99232378843586
H	1.37738544580321	8.17556449679428	5.78710101058385
H	1.44360721859256	8.69221656403568	8.22396438293821
H	2.61528210272281	7.14282072929686	9.80386619661629
H	3.72694612967822	5.08018589983902	8.91951494379917
H	3.66597047630514	4.57283531164366	6.49307655285229
H	1.48530660918588	-1.40848484090821	3.79457772095985
H	0.72441516034808	-2.83288077600752	5.69294540920446
H	-0.95081123967732	-1.94996031531786	7.33120082492182
H	-1.86178261529069	0.36527074827360	7.04500495836170
H	-1.10740257483191	1.77744760828420	5.15138125462703
C	4.91868016516749	-0.25830275180957	7.65531207484476
C	3.39438787729955	-0.09606414821858	10.12559573498792
C	-2.26622090272282	4.71998887322467	10.16970293017557
C	-2.97789170940578	5.88520617229367	7.60021052392275
H	1.33461251774371	1.33963417310640	11.10360006281143
H	-0.52413432120456	2.89701197132517	11.11273645658923
H	-1.07682712803112	7.47301610839179	6.08097384926716
H	-1.57859657137503	8.58268073849807	3.90654235281788
H	-1.95476570941749	7.20261274576776	1.85119973157893
H	-1.83236283936501	4.70540608624647	1.99676618222547
H	-1.33818529017589	3.60449261267085	4.16301903056175
H	3.67854606251166	-1.05176252695105	5.16274207411650
H	4.88116121701137	-1.30032490589162	2.99425513444379
H	5.76277469416988	0.72185692958184	1.80940267623235
H	5.43547460130358	2.99001452841739	2.81955080540594
H	4.24301950810377	3.23326301685832	4.98002982647967
H	3.73223520054864	-1.10599132821518	9.84115036542388
H	2.59660938535664	-0.21660056540708	10.87310337954162
H	4.24855286449538	0.39501272827872	10.63153450589177
H	-2.57463669506619	5.77794932265469	10.18801575924243
H	-1.73312704269637	4.51858173847454	11.11065242448485
H	-3.19490354505037	4.11646175715601	10.18183469008550
H	1.55963165209925	1.48061542055883	-1.33078556618538
H	-0.15170445142989	1.09195963101498	-1.04633799875213
H	1.10259978704815	-0.11131380824008	-0.69622711279801
H	3.01126680493231	7.54602747885943	0.17454673427739
H	4.54512913119301	7.66607062160631	1.06566527763840
H	3.18657760870720	8.72453058540006	1.48837325984374
H	5.52053931020536	-0.04861034276319	6.76024074287496
H	4.70981467278393	-1.34524686327039	7.66593175534033
H	5.54518857850231	-0.04866117820716	8.53972106945350
H	-3.26536047776087	6.06212391381630	6.55451025302172
H	-2.84686814037314	6.87479365545611	8.07844858755896
H	-3.82999089646070	5.39968065642152	8.10699346828299
H	-0.89548831267150	-0.51101666746307	0.71184311352955
H	-0.73167808281530	-1.02310329447671	2.40869365756242
H	0.53436482272242	-1.42334813697926	1.22733177577451
H	4.63168154695506	8.41600657548230	3.46479929308420
H	3.93380524510179	8.23154206578406	5.09167535535939
H	3.05783219084494	9.14049358883802	3.84078985246029

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Heteroleptic phen-POP reduced

Cu	9.73862008120407	0.35173027096576	2.85941043415696
P	10.29649135949230	2.51920195726702	2.88013404231595
P	10.40658280382485	-0.81301258964225	4.66651679226767
O	12.65117059048898	0.98335453058077	3.66388494112455
N	10.24050354617964	-0.68116816445824	1.14580579006313
N	7.83268015653309	-0.07110609481482	2.18241562659422
C	11.44967592312294	-0.94519687291098	0.62602308608846
C	11.63274729103703	-1.71415336999733	-0.54301315955436
C	10.51972079246784	-2.22477696974628	-1.20528063758466
C	9.22389525483886	-1.95458762271427	-0.69529011006824
C	8.01018137537340	-2.41925719747052	-1.31357672743315

C	6.78056734253498	-2.10516811868504	-0.78640587438629
C	6.66286316065635	-1.30177500295871	0.40209667129864
C	5.42079911905449	-0.92719074454438	0.97486027243281
C	5.41191509502159	-0.12906540825911	2.11478560586316
C	6.63749187684690	0.27719949359498	2.68314383910761
C	7.84898146012739	-0.84124422887357	1.04916426872221
C	9.13958677008162	-1.16934352008991	0.49406408005640
C	11.46879654434331	2.97204690941100	4.22363817581260
C	12.51532019549866	2.07137361458454	4.52781388301938
C	13.39372313086287	2.30189124678060	5.59597325956382
C	13.24571721118401	3.46672492996795	6.36320477270248
C	12.23601922045733	4.39368638868121	6.06231405806195
C	11.35566499571490	4.14429498685605	4.99992439246849
C	8.88027156524812	3.67356322969203	3.13141890386582
C	8.1380350069015	3.55738474933316	4.33014198749826
C	7.01377115182132	4.36602701072247	4.54868296509870
C	6.60617452144382	5.28807585413882	3.56932710819063
C	7.33518034807033	5.40337245096837	2.37663347421362
C	8.46933707142683	4.60424034544185	2.15670843088334
C	11.12225688131336	3.09578928802928	1.33616057398671
C	12.28435311281205	3.89417627501774	1.35246809247463
C	12.87473437282649	4.30722653753582	0.14807919873295
C	12.30732760961262	3.93852691453414	-1.08154368003320
C	11.14757215177054	3.14678545095952	-1.10653082751515
C	10.56335393150577	2.71868069088746	0.09451351236540
C	12.22066939381937	-1.17895336368263	4.67616982724694
C	13.13580196800494	-0.22792678020407	4.16630899906057
C	14.50564451760379	-0.50634247083655	4.05858816790100
C	14.99494201246364	-1.74500043622110	4.50029603248673
C	14.11275020899834	-2.69539278512011	5.03714198730786
C	12.74016351146459	-2.41644174968341	5.11600801034693
C	9.66239971177866	-2.50102183747332	4.77656806933128
C	9.81036812326061	-3.35610587588113	3.66026602199242
C	9.24224719099639	-4.63684284229311	3.66674624941400
C	8.50643625205907	-5.07636686782730	4.78034320034713
C	8.35212973613691	-4.23187105951984	5.88937783095827
C	8.92906586500593	-2.95108231601021	5.89280115898779
C	10.06229787387854	-0.06793468826693	6.31492061274702
C	11.03079835189026	0.04089793577576	7.33203966059229
C	10.69303099315576	0.60837074621498	8.57092975405742
C	9.38641901420866	1.05883598597326	8.81195668312898
C	8.41114271258747	0.94328550597670	7.80737393781590
C	8.74866980897046	0.39077618279316	6.56336002451137
H	12.30455028805686	-0.52439386331600	1.16409732595002
H	12.64455298888964	-1.89608514431202	-0.91550675483307
H	10.63102757325417	-2.82446540322283	-2.11486738452380
H	8.08499042647991	-3.02683127980689	-2.22156863952435
H	5.86404662464822	-2.45950074581236	-1.26972328785289
H	4.48605551840852	-1.26110380457048	0.51237380765393
H	4.47259910772244	0.18878579149997	2.57537045191121
H	6.65665489637397	0.92036229737078	3.56897599457382
H	14.19011150163265	1.58526231655864	5.81495205625885
H	13.93480346589230	3.65232060182689	7.19336646690989
H	12.13114398057775	5.30794465545001	6.65409711123577
H	10.55643384849461	4.85683433431507	4.77547264589114
H	8.46210068478737	2.85223240754594	5.10570923796856
H	6.45658370523255	4.28001617913285	5.48775456313794
H	5.72647749691584	5.91717187495684	3.73934269081481
H	7.02785827445408	6.12557978979963	1.61307281809936
H	9.03609810986046	4.70932655183633	1.22671077512556
H	12.72682379470687	4.19404440515913	2.30743502458130
H	13.77820140584727	4.92544124443043	0.17237381187961
H	12.76764146102059	4.26693285353299	-2.01905469362790
H	10.69957947541227	2.85740599082971	-2.06296924260513
H	9.66353189214932	2.09322499397576	0.06940069815171
H	15.16933109116494	0.24885596360449	3.62684014587798
H	16.06443140155921	-1.96443549431304	4.42260505952219
H	14.49055224019263	-3.66090907409415	5.38736799167417
H	12.05460915221098	-3.17221160910315	5.51092909524632
H	10.39022710950433	-3.02209690690390	2.79248316699571

H	9.37280146031232	-5.29361237789501	2.80020364224576
H	8.05845846427096	-6.07526834650204	4.78326222906406
H	7.78613144375857	-4.57082404738579	6.76334649897869
H	8.80983075292457	-2.30539959796598	6.76766930767976
H	12.04889372431982	-0.31944501572495	7.15746303883507
H	11.45458817718802	0.69129047925904	9.35317447174575
H	9.12595352957945	1.49583292797615	9.78122985580265
H	7.38680059987437	1.28261293714183	7.99373732488095
H	7.98224407054990	0.29112361022681	5.78491924358518

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Heteroleptic phen-POP oxidized

Cu	9.72918172778179	0.24580316887246	2.82525455655583
P	10.16145012648619	2.49848514748059	3.09700060293957
P	10.53398596662653	-0.83496976256282	4.69298845410820
O	12.60677458033122	1.05437075666443	3.69323852408783
N	10.26385453856953	-0.99395800781989	1.26509861569659
N	7.92534644563932	0.21522449965008	1.85357588834652
C	11.45938091840062	-1.51035230405681	0.94380899611049
C	11.65961398852041	-2.32112189182019	-0.19519086671910
C	10.57718145691738	-2.62098341159831	-1.01626913776108
C	9.29837206551409	-2.08367190824138	-0.71109397080157
C	8.11941026483956	-2.32756889122867	-1.49963371122809
C	6.91222872145269	-1.76217344301066	-1.16283013263080
C	6.79212625569029	-0.89093746610250	-0.02329819416901
C	5.57991872306324	-0.25732201443027	0.35981147875087
C	5.56914398748197	0.58846322957668	1.46383869196779
C	6.76669685194144	0.80932915940372	2.17875920531556
C	7.94419425647289	-0.63026731451747	0.77516212045842
C	9.20130852327465	-1.25164623227711	0.44337964043979
C	11.36726776313437	2.95817593995069	4.38128750942707
C	12.49144535928831	2.12311688460606	4.58335342346497
C	13.43981239973063	2.40422062378486	5.57459412790433
C	13.27282215224280	3.54829588227009	6.36993430767147
C	12.17638277030112	4.40460940161158	6.17475705215808
C	11.22759347825310	4.11007989796280	5.1879798404640
C	8.70290046881353	3.56682851821253	3.36356904604604
C	7.99455659811293	3.43015224730197	4.58288291750983
C	6.86443023279875	4.22126533145152	4.83068336973860
C	6.42481945627114	5.14559600953802	3.86614558137654
C	7.12501867296353	5.28389107515805	2.65707553925278
C	8.26045451640984	4.49989610962037	2.40027897853189
C	10.88726668274336	2.93611147385252	1.47487502639178
C	12.16771203125219	3.52468594256297	1.38036069935467
C	12.69178366453560	3.85902964748172	0.12374219239474
C	11.95312070076220	3.60492153206328	-1.04360091871881
C	10.68158328659500	3.01236890820298	-0.95614278699258
C	10.15169550483428	2.66817071708034	0.29429486858200
C	12.33687305013159	-1.15753217791919	4.61445467558992
C	13.19082407244592	-0.14113913972264	4.12339080800008
C	14.56750284649913	-0.34788018518854	3.97187243065209
C	15.11910357462607	-1.58113891142513	4.35687338577951
C	14.29611392119088	-2.59428867623356	4.87558283584871
C	12.91332034916724	-2.39007841694895	4.99484636093938
C	9.74527939584883	-2.49071827542194	4.79147541872957
C	9.98491690156221	-3.42446112661842	3.75357818280957
C	9.39531164651209	-4.69361342964547	3.79690850945664
C	8.54724244563750	-5.04238068923192	4.86265745983879
C	8.30037100819142	-4.11914763982512	5.89076518424137
C	8.89182207295358	-2.84770287074363	5.86005686184071
C	10.19391247245939	-0.01710097105170	6.29186572113224
C	11.18605091496389	0.12671812182851	7.28390198205946
C	10.85761284701445	0.69433952928868	8.52445812874966
C	9.54392823725320	1.11265612502009	8.78738684946576
C	8.54910728901023	0.96528846003903	7.80513866530227
C	8.87163304366824	0.40995777312891	6.55849386785809
H	12.28749361311157	-1.27755157768306	1.62069999360271
H	12.65798761617961	-2.71043788108928	-0.41084999161718
H	10.70120013586321	-3.26178743905217	-1.89545642156295
H	8.20079468921000	-2.97533625824141	-2.37818526302735

H	6.02106635395904	-1.96010452204746	-1.76673225627840
H	4.66810933663190	-0.43411831819786	-0.22006117063518
H	4.65346895326997	1.09454058402255	1.78005234128922
H	6.79477039903491	1.49845205878073	3.02899796328744
H	14.30179259446199	1.74712180535027	5.71727013151712
H	14.01655269781999	3.77647978183447	7.13960805444328
H	12.06334665391211	5.30379371791491	6.78680137024667
H	10.37167815067536	4.77381829911500	5.03776422394645
H	8.34900687919807	2.72842398280990	5.34651471841888
H	6.32964671511268	4.12388280695017	5.78076870736943
H	5.54347098702146	5.76386432866419	4.06260298417518
H	6.79556129061935	6.01525323290085	1.91255140300385
H	8.80837519147635	4.62910332997239	1.46291463570661
H	12.74227665506633	3.74155351026321	2.28511534230523
H	13.67718342553435	4.33050141294155	0.05770737536626
H	12.36576444924181	3.87230359838772	-2.02124092079435
H	10.10116188288381	2.82138631099236	-1.86419683709988
H	9.15489599016357	2.21810163570841	0.35553632311349
H	15.19015244607881	0.44866367449047	3.55411460728106
H	16.19523371754713	-1.74768024948636	4.24983664044993
H	14.73010606218471	-3.55024819025921	5.18286530901884
H	12.27464287616715	-3.19053235725996	5.37933792449493
H	10.65456556634842	-3.16829886608498	2.92713108195485
H	9.60041319986537	-5.41522270468912	2.99993338812700
H	8.08554916903911	-6.03402971419135	4.89341724528339
H	7.65277429569277	-4.39142968541542	6.72984916058481
H	8.70592824383395	-2.14719413484883	6.67817491935316
H	12.20778098839072	-0.21431028409539	7.09421571065277
H	11.63029837351950	0.79828932212665	9.29237017654141
H	9.29145582541898	1.54584284086060	9.76003051237814
H	7.52021363592824	1.27429569903889	8.01521694894543
H	8.08729971235519	0.27792329349325	5.80285466025633

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Heteroleptic phen-POP triplet

Cu	9.68856920096011	0.16462832139308	2.72922551126811
P	10.09552694570705	2.43665527265924	3.09666916462191
P	10.52680523233810	-0.89064451850125	4.63717942220888
O	12.59125475731659	1.03289892341832	3.63973207712795
N	10.20713346963760	-1.18308770821224	1.36120985584584
N	8.01017026344379	0.30575640701908	1.67486403291855
C	11.36255636565951	-1.87693827916579	1.17908207810964
C	11.58677021550138	-2.71169343141812	0.08526968233385
C	10.57183261824458	-2.88219628218555	-0.88693366073454
C	9.36079951515844	-2.18243624797772	-0.74158035351710
C	8.24966873037386	-2.27455601535855	-1.65631835095844
C	7.08680330827381	-1.57040600901007	-1.45089413076857
C	6.93046608521721	-0.68096730442723	-0.32679992136029
C	5.76927251404874	0.06416897756324	-0.05800748883324
C	5.73816592244730	0.90284266125688	1.08154818653205
C	6.86466761307767	1.00225730458611	1.89826548432729
C	8.03872725920085	-0.56019961256702	0.57645277212251
C	9.21105073266495	-1.31439551182391	0.39062811745219
C	11.32516227999492	2.90599356076764	4.37200616695861
C	12.47165650353784	2.09520279078049	4.53460347790916
C	13.44568643170235	2.38960665840425	5.49870325755777
C	13.27800840803154	3.51646566609170	6.31723640594219
C	12.15419618387122	4.34431585816334	6.16801375659072
C	11.18727231374796	4.04076796271995	5.20007917151307
C	8.66647004116667	3.54003713173507	3.41844764162421
C	7.94712302366971	3.36206921795997	4.62340327669710
C	6.83011377870990	4.16236219609707	4.9002777968497
C	6.41396284710526	5.13684354369900	3.97668717364650
C	7.12370896668143	5.31393702912162	2.77910317520921
C	8.24789995764213	4.52190679696839	2.49688719265836
C	10.82792613901123	2.98383066033058	1.50066209479370
C	12.00414659263318	3.76302824913248	1.4582432235247
C	12.53125807201347	4.17159638230390	0.22456215999090
C	11.89347479978419	3.80997195622665	-0.97256012701628
C	10.72273815402321	3.03554944435453	-0.93585825861921

C	10.19333654660639	2.61455543316099	0.29225058798173
C	12.34467186312655	-1.17209575780003	4.59583859174838
C	13.18221735548373	-0.15805429545791	4.07240707074490
C	14.55391336739906	-0.36380305652904	3.87913936464295
C	15.12111892812919	-1.59434536828318	4.24700495337315
C	14.31474077357694	-2.60869139963008	4.78770905735186
C	12.93646896594123	-2.40418537772272	4.94977076532805
C	9.77422250358823	-2.55120184203748	4.90089023306166
C	9.25700307226195	-3.27861040623848	3.80759481612741
C	8.69447218497266	-4.54805395028122	4.01019204163316
C	8.64114090889446	-5.10095036151950	5.29844908220297
C	9.15000461869507	-4.38034760407111	6.39177326598880
C	9.70943842726134	-3.10947229538174	6.19960017348436
C	10.15322217650142	-0.04692170438737	6.22488451510779
C	11.13738960183183	0.31035279085018	7.16672785056931
C	10.76418988217823	0.90948051866757	8.38058870396071
C	9.41124927291632	1.14633812046331	8.66700797633596
C	8.42350038170247	0.77886240549881	7.73688915059656
C	8.78981919604538	0.18807771870094	6.51948555084848
H	12.12289990067582	-1.75629161677540	1.95659539318835
H	12.53946898218202	-3.24099178426625	0.00357397104744
H	10.71886389815943	-3.55264308905706	-1.73943163428481
H	8.34836894263900	-2.93189772782367	-2.52712600391231
H	6.25011906863779	-1.67342587846680	-2.15050544148008
H	4.90584618117762	-0.00550432136480	-0.72705924753997
H	4.85134177226789	1.49423551595542	1.32237293282367
H	6.87160875754634	1.67439907093821	2.76148804031302
H	14.32479923853874	1.74791984618004	5.60387999723533
H	14.03969090411364	3.75145935798954	7.06748497940742
H	12.03207735455463	5.22898791293878	6.79979829069915
H	10.31068284128833	4.68435293484895	5.08514490162182
H	8.27152512212770	2.60533992981233	5.34726178161937
H	6.28198382738532	4.02427680040885	5.83793717525579
H	5.53852876373629	5.75757289905602	4.19245645233410
H	6.80601533600863	6.07555998228235	2.05979961103184
H	8.79765680635606	4.66783926952165	1.56262481506567
H	12.50335359853757	4.05583520206254	2.38644602964820
H	13.44211297877437	4.77852286612866	0.20065019524394
H	12.30895878218500	4.13030419201857	-1.93335010124446
H	10.22179176978188	2.74965642382934	-1.86615820272703
H	9.28150078188456	2.00955721079567	0.31238197853665
H	15.15697571413995	0.43222936766863	3.43269013903701
H	16.19296854089903	-1.76044102297678	4.10161218043199
H	14.75632261480012	-3.56874331436013	5.07136580345911
H	12.30723530109954	-3.20980288322416	5.33994565806648
H	9.29181899578152	-2.85215605504700	2.80187974189867
H	8.29181275853422	-5.10163166050617	3.15607115120916
H	8.19803761391811	-6.08994105926807	5.45335876940352
H	9.10683806619510	-4.80572047028913	7.39963857382034
H	10.08855460905210	-2.54747771619726	7.05885927800852
H	12.19274754504002	0.11181556722405	6.95935527447999
H	11.53540900744360	1.18117667943759	9.10836007925423
H	9.12423759580471	1.60610366666639	9.61801181306343
H	7.36507908461157	0.94186752987720	7.96502049670967
H	8.01338167441148	-0.12323924612521	5.81018132917851

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Heteroleptic dmp-POP reduced

Cu	-1.18103702759222	2.92078854189032	11.15942125337944
P	-3.35893592066617	3.56220328051173	11.12640218262092
P	-0.61111504562910	1.05043308922219	9.99733981303944
O	-2.75002414217860	2.28075171666657	8.44315069012260
N	0.12073198984917	4.48165826837070	10.71947386237390
N	-0.30330993667669	3.14484214074385	13.04942629665919
C	0.28698749413806	5.15771967683741	9.56362359474812
C	1.31128928965931	6.12960080105752	9.41561068365413
C	2.16805110780815	6.40987832163214	10.46871578836396
C	2.00446847578047	5.72435721395830	11.69847301725512
C	2.83702990901840	5.96394529609224	12.84378497700689
C	2.62427646556604	5.28864955843056	14.02021385598784

C	1.56415331881220	4.32653614070287	14.13469687082542
C	1.28975879811750	3.62403863251100	15.33601870280332
C	0.22853365864224	2.73594760049011	15.37249613657306
C	-0.56350666258755	2.51840209092732	14.21297026706843
C	0.72834143646161	4.05024129850830	13.01104659740892
C	0.95160223005836	4.76115020313139	11.77300971848789
C	-0.65482779300290	4.85894438608469	8.43136245519093
C	-1.73776355246323	1.58065505089711	14.28153703506048
C	-4.16278978615685	3.93912996187711	9.49618980271481
C	-3.78447092952973	3.21553631355049	8.34306130685212
C	-4.34893489347545	3.48125019373468	7.08662469127742
C	-5.35003540078383	4.45627625811783	6.97247192083778
C	-5.77317686021442	5.16242700066109	8.10982886688552
C	-5.18216256982799	4.90671031544417	9.35505047666146
C	-3.43695741064948	5.16037738617393	12.04025875313824
C	-3.55228479342948	5.14798332124438	13.44847824419799
C	-3.45016482411555	6.33843668624461	14.18285581092366
C	-3.21512766857019	7.55697281736455	13.52672112372786
C	-3.07538772784202	7.57626362985455	12.13036181027009
C	-3.17680802516131	6.38771426037445	11.39194910315523
C	-4.66202095882578	2.51266162782808	11.92247115488817
C	-4.52410911986160	1.10973284994997	11.86758623489676
C	-5.52302481644753	0.27467790460503	12.39268185169174
C	-6.66931065004141	0.83116637030727	12.97914049625018
C	-6.81996188964158	2.22681011833728	13.02903516154034
C	-5.82798887894396	3.06357348625474	12.49805551656151
C	-2.04078173686290	0.16404240082479	9.23950814103903
C	-3.04879805522737	0.93223305744788	8.60734515163947
C	-4.23780638085621	0.34659955580730	8.14895716542059
C	-4.41166678887122	-1.03921133585480	8.27814529666041
C	-3.40595705667481	-1.83246660072235	8.85096175357112
C	-2.23220565804194	-1.23127979491327	9.32851662879759
C	0.53291367377426	1.37449092600035	8.58768981343579
C	0.25006846229766	0.95515305630878	7.27155018163882
C	1.14974177794890	1.23514867496185	6.23093982451796
C	2.34451864134044	1.92308053790442	6.49312108386796
C	2.63788766011790	2.33759039646170	7.80278708902465
C	1.73462518834962	2.07402672739248	8.84284471815157
C	0.23740091432174	-0.27993643446138	10.96229230790955
C	1.54821234379216	-0.71856256640040	10.68694377424786
C	2.15196758915362	-1.69936814712951	11.49099203479821
C	1.45415037960961	-2.26351206766995	12.56858484195804
C	0.14197475055870	-1.84251749115565	12.84238131579437
C	-0.45784416269659	-0.85347611229305	12.05104673337997
H	1.41138103985669	6.65176178142390	8.45993194189549
H	2.96261553449161	7.15671941421129	10.36529471414270
H	3.64200960098839	6.70167428929703	12.76083790487812
H	3.25624848035974	5.47694998411376	14.89439049532727
H	1.91012195065784	3.79934307392315	16.22145850843376
H	-0.01653321349944	2.19304276975313	16.29036458242579
H	-2.26344430444370	1.54647569629348	13.31643348315497
H	-2.45448568599553	1.90702502928801	15.05661956565004
H	-1.41328327823460	0.55982918479813	14.54910210219385
H	-3.99459896344311	2.92430634133168	6.21414173648468
H	-5.79727037095167	4.66275229040634	5.99512950338212
H	-6.55985258935318	5.91870168605065	8.02727999903908
H	-5.50298298799127	5.47708668769751	10.23213248508600
H	-3.74050292320218	4.20384679140663	13.96988880018010
H	-3.55937494084525	6.31296661293671	15.27220335112540
H	-3.14039515576661	8.48612724812861	14.10059862211999
H	-2.88978046430413	8.52158876901463	11.60967963760371
H	-3.06977943990555	6.42093654302040	10.30299680969669
H	-3.64167129902153	0.66488535440100	11.39379713501958
H	-5.40345618737972	-0.81227976930942	12.33961748011825
H	-7.44667638763688	0.18045239536264	13.39255828190162
H	-7.71602183642405	2.66704303904773	13.47883795853522
H	-5.95596701533541	4.14961954864843	12.54398833135721
H	-5.01428701660964	0.96490458366255	7.69143331460426
H	-5.33759507495644	-1.49758800685736	7.91642637458915
H	-3.53416724688017	-2.91616257531421	8.93063201154492

H	-1.45796757003585	-1.84682661447708	9.79485083579055
H	-0.59239498521210	3.79811646793936	8.13500329393997
H	-0.43170148964080	5.48183996498484	7.55106925274899
H	-1.69935334945407	5.04827667532169	8.73483931824954
H	-0.67146587996385	0.40407080361721	7.06092431501125
H	0.91893013028611	0.90456730048064	5.21285896982573
H	3.04697247060661	2.13360889309053	5.68022857733747
H	3.57114261127838	2.86949611821795	8.01537256524790
H	1.96720357654304	2.40346987808310	9.86179163854363
H	2.09998220925492	-0.30080477619137	9.84020963952942
H	3.17080496930481	-2.02979368136987	11.26339756553776
H	1.92588494608209	-3.03247750961649	13.18869399490251
H	-0.41672681408351	-2.28920859707844	13.67197353419598
H	-1.48560948077044	-0.54025227883821	12.26426738769537

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Heteroleptic dmp-POP oxidized

Cu	-1.05687277519019	3.04572495627982	11.17112735466652
P	-3.33373890294811	3.46838761510599	11.21091214211844
P	-0.75091735623970	1.05557463255484	9.98997754043391
O	-2.82385784904157	2.39405385202375	8.54149689633147
N	0.28715247376770	4.50602452445266	10.48228832907748
N	-0.06574125840781	3.44440953076142	12.97974324510312
C	0.40104936799254	5.07680118061191	9.26168396284841
C	1.43477341109628	6.00909568199509	8.97773711516987
C	2.35196481326255	6.35721984906241	9.95472004643296
C	2.23659653550059	5.79393183926701	11.25183128540590
C	3.13042661860650	6.13135659133861	12.32338194446180
C	2.96000288028656	5.58937151194521	13.57311084992857
C	1.88196523198045	4.67804924748673	13.83501063776998
C	1.64809259047760	4.12248686770808	15.11894065908981
C	0.57283552364782	3.27009491788782	15.30501733204037
C	-0.27878581592215	2.94695947996127	14.21643683762546
C	0.98575692993281	4.30433026564861	12.78739786068180
C	1.16988226854769	4.86920973048767	11.46930581532085
C	-0.61016078883425	4.73549794965106	8.20625909925247
C	-1.44835105493934	2.02800664006306	14.42091422272857
C	-3.97229349237011	4.18057048487571	9.64273139028506
C	-3.73869424527855	3.44440674267200	8.45774191171485
C	-4.26543385913514	3.84251884730456	7.22460146910472
C	-5.06095470114649	4.99954351035370	7.16987588213332
C	-5.30306281761978	5.75089356499234	8.33209080600888
C	-4.76117296042261	5.34848533323487	9.56298991169235
C	-3.53065344782227	4.79520759368979	12.45514644155899
C	-4.29706955040859	4.60002817096418	13.62618336095053
C	-4.39719114549306	5.62868723553294	14.57450969753062
C	-3.73505616822497	6.85028056160979	14.36765473947681
C	-2.96671558805395	7.04756463515674	13.20638253476716
C	-2.85486993439630	6.02453293879683	12.25639237177366
C	-4.59001164568299	2.19273976004677	11.61779533867201
C	-4.24265199372599	1.04330392677607	12.35631530195197
C	-5.22539603514554	0.11546786985252	12.73219161942301
C	-6.56531707115012	0.32623087904457	12.37120267524842
C	-6.91998273574364	1.46702528675850	11.63245636588043
C	-5.94149398514541	2.39616841197637	11.25303706813193
C	-2.24515418658842	0.25009608145893	9.31696940172154
C	-3.20750776534424	1.06791242829183	8.67562206566750
C	-4.40783474165896	0.54495440214895	8.18107318670810
C	-4.63713943273194	-0.83434077046600	8.29111207360415
C	-3.67628927313098	-1.67847105488132	8.87521670049839
C	-2.48972995215683	-1.14034397345061	9.38858194635052
C	0.39773123192247	1.28447492973496	8.58049829398680
C	0.07325989440951	0.78838783649458	7.29773751913541
C	0.98601622198824	0.92654285384185	6.24183598717583
C	2.22365448885898	1.55510424716778	6.45221051069299
C	2.54982463911756	2.05494530199821	7.72468797470997
C	1.64004905847784	1.93117653425431	8.78382902245566
C	0.02322087120760	-0.17991206973029	11.10591101311162
C	1.39918220395905	-0.49591356405211	11.03584279546659
C	1.95344369961490	-1.42582271508049	11.92726911267097

C	1.15117268547990	-2.04807367492760	12.89735024738164
C	-0.21929156746198	-1.74289884602103	12.97195250905138
C	-0.77913659577822	-0.80821916664340	12.09165725922715
H	1.49318693945554	6.44446688196231	7.97669403148361
H	3.15678647126022	7.06882519183159	9.74195288012772
H	3.94416773353245	6.83611499584021	12.12556360242631
H	3.63682669488991	5.85047164043566	14.39267630594260
H	2.31192963484789	4.37968705338336	15.95099279699410
H	0.36449630029916	2.83967870895159	16.28802196371366
H	-2.38256224775714	2.50216988200588	14.07387922344627
H	-1.57214430759858	1.76635421961168	15.48293660555987
H	-1.29951539220967	1.08988479678764	13.85605811425649
H	-4.03498422585509	3.26775774404382	6.32292489842233
H	-5.48053821171981	5.32037993775395	6.21169224876770
H	-5.91912747019049	6.65350497096845	8.28215645153021
H	-4.95457956397197	5.93637235937814	10.46497809574366
H	-4.83194728754626	3.65842173936223	13.78263351720537
H	-5.00557969561870	5.47954356050541	15.47192768616746
H	-3.82159441531033	7.65142053235743	15.10808262585725
H	-2.45863308028461	8.00255546628692	13.04002082877537
H	-2.26285660842077	6.18785633898975	11.34874262279813
H	-3.20244497623138	0.87551277357754	12.64427901340630
H	-4.94529590804302	-0.77243570370955	13.30760612463091
H	-7.33247014898745	-0.39659137253284	12.66543841172584
H	-7.96396859754558	1.63732121323616	11.35148506812223
H	-6.23131498016069	3.27995638280653	10.67707269169766
H	-5.14360855122492	1.20150057729047	7.70913925766600
H	-5.56870002992899	-1.25394524591600	7.89926611912893
H	-3.84991171960187	-2.75702703449896	8.92597103141635
H	-1.74534519170923	-1.79856236706210	9.84471521479728
H	-0.69871209096646	3.64599085848290	8.06521709700755
H	-0.34200544821060	5.19040718718873	7.24067709379495
H	-1.60639784366958	5.11579389530075	8.49442852660702
H	-0.88072870910799	0.28137954678586	7.12839705788377
H	0.73158525593167	0.53075250671371	5.25376773854288
H	2.93512388943634	1.65389094958543	5.62662741869931
H	3.51578251327235	2.54125236315251	7.89271726980954
H	1.90102964484082	2.33239309649823	9.76888527859812
H	2.03223851476637	-0.04450186731996	10.26785787403134
H	3.01595851925639	-1.67644764448380	11.85107449834048
H	1.58844036110985	-2.77769522288584	13.58569487592666
H	-0.85379583762815	-2.24180819420819	13.711123763704327
H	-1.85397288019455	-0.60587411657238	12.12802051949662

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Heteroleptic dmp-POP triplet

Cu	-0.98226655115065	3.06675431375508	11.16725263347907
P	-3.31273997970421	3.42888089781869	11.30366289905280
P	-0.67176275988130	1.11759777111308	9.88102744849358
O	-2.80875738417537	2.41844783065393	8.52201122844029
N	0.34005427293684	4.40385181434840	10.47877966723926
N	-0.17314963575513	3.47172204628394	12.96530132690254
C	0.48920157702941	4.99691306595205	9.24880075171137
C	1.53599190932723	5.88822032392162	8.98706775391475
C	2.48329721371454	6.20492564374543	9.98471090696883
C	2.31941887312849	5.66965771923942	11.27399286186953
C	3.17829879295618	5.98962306387244	12.38210759537802
C	2.94030760972048	5.48392620306626	13.63826183728375
C	1.80950284697273	4.63539011796748	13.89821033965199
C	1.50036187319759	4.12608995005743	15.17015232122560
C	0.36475159737455	3.30658879062068	15.32139911847881
C	-0.45148315855619	3.01051486283166	14.22143648148059
C	0.94814640954349	4.29159116260823	12.80048327052877
C	1.21310007632570	4.78350385605728	11.50583382875792
C	-0.53862024833157	4.70237050829959	8.19322571394463
C	-1.66102703976883	2.13630476869565	14.39839755974376
C	-3.96427094113909	4.15267047989243	9.73122868444873
C	-3.72569854735214	3.47019724788268	8.51646891265299
C	-4.25227945290556	3.91951709914110	7.29993117985458
C	-5.04816839081441	5.07614694058225	7.28437034477479

C	-5.29197927469450	5.77827270442853	8.47499701851178
C	-4.75244126499597	5.32257544096479	9.68828848061534
C	-3.57563095853710	4.77886984689407	12.52394612940552
C	-4.54325305933341	4.70162167390123	13.54728160625702
C	-4.68025802143802	5.75577309991675	14.46475482237122
C	-3.86046894903495	6.88993704599613	14.36672300427714
C	-2.89338806001525	6.97041433159370	13.35023464642541
C	-2.74273285382352	5.91861424000471	12.43720349819182
C	-4.60772378443051	2.17041023685902	11.68549311203619
C	-4.26222777621904	0.95555132897033	12.30930361442526
C	-5.24799118660769	0.00799835547357	12.62354901778253
C	-6.59235742404946	0.26295760086685	12.31390188538024
C	-6.94759034004258	1.46916483944418	11.68813644180594
C	-5.96425353000048	2.41700341602793	11.37209464349211
C	-2.19023426786001	0.28084588017039	9.28613632153678
C	-3.19031464953244	1.09955083093617	8.71082527637861
C	-4.42946651982987	0.58282469267062	8.31207878219675
C	-4.66216565568014	-0.79297794767030	8.45144260361381
C	-3.66664918719582	-1.63957763225075	8.96805041361600
C	-2.43953630851646	-1.10513735934008	9.38451056047587
C	0.43391521945010	1.23747078038998	8.42043044500805
C	0.11701701183877	0.58977442194234	7.20715411660814
C	0.99654581134697	0.67062471044432	6.11730899153731
C	2.19726584536695	1.38910955371701	6.22820091209805
C	2.51699942991512	2.03655983560574	7.43256293405224
C	1.63865658128533	1.96969956739206	8.52383464614125
C	0.13400368627522	-0.09540493138519	11.00940574358504
C	1.52197792567924	-0.34736087233376	10.95463329568185
C	2.12094857050093	-1.21145079675406	11.88304499093256
C	1.34986994166793	-1.83265592429166	12.87763495377802
C	-0.03189581248247	-1.58925364338889	12.93996256919214
C	-0.63481843268520	-0.72009935478348	12.02065867585024
H	1.60976470424141	6.33106486244840	7.99024861700097
H	3.32095203736106	6.87650978636791	9.77160840502392
H	4.02565824752521	6.66103581574099	12.20520882297614
H	3.60712269049372	5.73054121896247	14.47168008389313
H	2.12964605497805	4.37840670546194	16.02962692845914
H	0.09423846345662	2.90497495069352	16.30140832798240
H	-2.56560253657630	2.60674281549151	13.97590641298747
H	-1.85042279441648	1.93426420328584	15.46427598668904
H	-1.50918206781477	1.16432172408602	13.89205241804739
H	-4.01313893852247	3.37857524141303	6.37970785333008
H	-5.46255228422693	5.43511434139481	6.33729288449314
H	-5.90111534467936	6.68719909985607	8.46175177480699
H	-4.93746500669330	5.87928329000755	10.61175749268225
H	-5.18997020917909	3.82282029673253	13.62756937415393
H	-5.43339959521320	5.68807271610876	15.25642157856079
H	-3.97133566200187	7.71008875930128	15.08318859817178
H	-2.24825900317305	7.85129581935850	13.27268301456574
H	-1.97661128607433	5.98424615968789	11.65626939451243
H	-3.21772177570084	0.75460475229857	12.55871791413838
H	-4.96394096902011	-0.93100961674048	13.10933559862561
H	-7.36192092942459	-0.47628325742585	12.55807942871868
H	-7.99507269217093	1.67444221846805	11.44436676019922
H	-6.25266379024038	3.35002229623498	10.87797959259024
H	-5.19062779745363	1.24577938452580	7.89156776690129
H	-5.62540779167424	-1.20704073047234	8.13727727710792
H	-3.84581648838848	-2.71589210252210	9.04707679710542
H	-1.66943771911214	-1.76239535572534	9.79852526995330
H	-0.66315827732718	3.62048832826482	8.02244258331281
H	-0.26138738972293	5.17207421062381	7.23657382895306
H	-1.52360837159279	5.10281235590833	8.49713316754788
H	-0.81262499835907	0.02033765087034	7.11508065098718
H	0.74281484657938	0.16506609986774	5.17996724955387
H	2.88171700813596	1.44769084228288	5.37588433564981
H	3.44793130085910	2.60498212672586	7.52324945535326
H	1.88170978798422	2.49968175726789	9.45008379826151
H	2.13476760749725	0.11497631708541	10.17610479478544
H	3.19652663550978	-1.40503151766667	11.82092319568040
H	1.82177207227010	-2.50782459042830	13.59827264791273

H -0.64329010477192 -2.07943115539500 13.70458962058933
H -1.71657930237590 -0.55915027126650 12.05767147819861

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Heteroleptic dbp-POP reduced

Cu 5.43041649324846 3.90160726273789 3.53675187941471
P 7.50490322409440 3.24312235739411 4.19777595444137
P 3.97524025855575 4.34796258092309 5.24992296581736
O 5.59021725895517 2.15417990780216 6.25280087811792
N 4.43496442067549 2.71335806984310 2.14630206805799
N 5.32719859562759 5.28519134958662 1.94114682346226
C 4.03320450352368 1.42706247325656 2.25414996203597
C 3.17354399946653 0.84283678485784 1.28744765824374
C 2.73235495190518 1.58289758875687 0.20224978120112
C 3.15116009748753 2.92855028193792 0.05940227670714
C 2.74110053703375 3.75826666869106 -1.03780109431582
C 3.17454078845049 5.05697303744956 -1.13306247641579
C 4.05322076145034 5.61220082700902 -0.14269865788439
C 4.53100600540393 6.94543928187526 -0.20881686160199
C 5.40840173482761 7.39549953515951 0.76095961002749
C 5.81399463745619 6.53699486526345 1.81931365779415
C 4.47890514463195 4.81820659836023 0.96579965276913
C 4.01422728228995 3.45281845035459 1.07101491959922
C 4.51500914208448 0.66051983110343 3.46572973478204
C 4.37502402488355 -0.87285938672336 3.44299428447635
C 5.29836926899538 -1.58489453618808 2.43725954271725
C 5.14013918305472 -3.11242392582028 2.45829206273849
C 6.84968277020876 7.02703683216520 2.80076549480074
C 8.21567003403965 7.31528546829523 2.12709996412494
C 9.28390326504098 7.85203939497316 3.10049364848945
C 8.98885730003807 9.25230340390660 3.66083228893591
C 7.64400896564342 1.62230498524660 5.09679369159391
C 6.69162484465756 1.30959461055256 6.09344505811993
C 6.75134847304169 0.11571573516481 6.82521324310580
C 7.79895580233198 -0.78679576577698 6.58627747682343
C 8.76283046948679 -0.49679295581266 5.60832248497914
C 8.68254650166804 0.69413403475728 4.87036187716257
C 8.58079726903518 2.97841737987443 2.72127920110665
C 8.25600152390186 1.92467271690701 1.83626256859366
C 8.97479342791842 1.74476884693935 0.64677243320075
C 10.01875864450377 2.62329149648747 0.31238188364848
C 10.33786033313952 3.68088799964779 1.17625500706006
C 9.62404123189621 3.86103810700708 2.37289296166545
C 8.51906545295674 4.31083471145523 5.32451140611197
C 7.92656619814713 5.40460365017532 5.98582909499538
C 8.67234065490264 6.18726594128534 6.88285226038551
C 10.01976302594100 5.88595782477894 7.12684446255853
C 10.61767452800818 4.78909949732092 6.48290831429596
C 9.87164528825122 4.00201831917509 5.59547873705813
C 4.74820672200463 4.25886829042109 6.92295788006845
C 5.59729833568759 3.16360425993162 7.20951296552906
C 6.33957828483973 3.09608703035301 8.39593589559947
C 6.21331639823325 4.12966514965971 9.33605161289796
C 5.35041994342420 5.21006475989251 9.09534950763521
C 4.62617633637909 5.27269054028127 7.89525587870956
C 2.55222696680539 3.17698450629535 5.32733369393405
C 1.71081388229514 3.07534090453102 4.19625698462030
C 0.61089129900060 2.20560038751738 4.20491656981431
C 0.34519305500265 1.41638260354400 5.33631161333747
C 1.17762968117289 1.51058419260198 6.46217239713942
C 2.27223776023505 2.38998587964694 6.46292471877682
C 3.15487653641667 6.00397135664636 5.27405992664903
C 1.77328971861549 6.17827297984030 5.49965798086812
C 1.21386613043923 7.46585378092258 5.51238976720479
C 2.02466101695908 8.59384169676475 5.31531701580781
C 3.40344259331177 8.43107961506671 5.10385666585361
C 3.96237590560589 7.14563631355139 5.07699160153508
H 2.86038429706018 -0.19632653674095 1.40863997237827
H 2.06792030334055 1.13984758633135 -0.54761086214260
H 2.07545598193817 3.33288665814710 -1.79616010696816

H	2.86143807685875	5.69150565968008	-1.96875875193760
H	4.21077833785333	7.59720240640326	-1.02876509563726
H	5.80533336877442	8.41417496425789	0.72388168156982
H	5.97297012717781	-0.09704243683286	7.56411048036187
H	7.85431699985412	-1.71792771048562	7.15881708993223
H	9.57833276638516	-1.20045102012724	5.41423208784122
H	9.42531730966473	0.90132678889634	4.09383777095220
H	7.44197613660385	1.23450706453833	2.08386846175078
H	8.71867753545626	0.91554485748754	-0.02093370078498
H	10.57953137829866	2.48282074373968	-0.61717890066888
H	11.15134368505736	4.36942780514912	0.92455617195069
H	9.89097948785386	4.68366330848242	3.04250625600935
H	6.86724760377240	5.63053142842524	5.82871117044327
H	8.19332239228141	7.02769828971256	7.39491932031141
H	10.60232494458672	6.49655322501302	7.82436056296956
H	11.66625094423178	4.54147886713024	6.67808850030833
H	10.34501402022336	3.14355496835717	5.10813346164316
H	3.98043304834385	1.06791597957977	4.34607549974056
H	5.57699492515726	0.92288047496137	3.62766751610277
H	4.61077720418824	-1.23847322360823	4.45981127822542
H	3.32031836779757	-1.16311403193459	3.26755279723116
H	6.34787031007274	-1.31737363016666	2.67117857169104
H	5.10868557362926	-1.20781976795891	1.41326764334836
H	5.35697140104970	-3.52265168254423	3.46098478836194
H	5.82470425312649	-3.59838585784070	1.74222507296455
H	4.11045986528770	-3.41309729784204	2.19277038368514
H	6.98069523954283	6.26783499325729	3.59049826200034
H	6.48119535513402	7.95193900285047	3.28436027929673
H	8.07586085124545	8.04340088015343	1.30444048028620
H	8.57432526273609	6.38103964063968	1.65758996685722
H	7.00318921190907	2.24699471739411	8.58072950576832
H	6.78902409229689	4.08030603519347	10.26576747433150
H	5.24122925225364	6.00527800741735	9.83904609093640
H	3.96891926321908	6.12460458484183	7.69879849003637
H	9.41053498353953	7.13727854079981	3.93644333183118
H	10.25152238942164	7.87712372822377	2.56459762611860
H	1.90811668332766	3.69295223593219	3.31280706712397
H	-0.04014769221798	2.14514957089686	3.32655581904848
H	-0.51174029902567	0.73500748273413	5.34193662718828
H	0.96950480986389	0.90556537668118	7.35087910865870
H	2.90449384748393	2.47016783556413	7.35208802124427
H	8.86417069992235	9.99045843464680	2.84768146733170
H	9.81548572904424	9.60191940970620	4.30269343037727
H	8.07085946121665	9.27131428612788	4.27518324735702
H	1.13237300197381	5.30779649770195	5.66558861775409
H	0.13935273439782	7.58564866902570	5.68581552368148
H	1.58539445583739	9.59652292278598	5.32947491674955
H	4.04371230943708	9.30747283439473	4.95697157188063
H	5.03861882622552	7.02779004719634	4.91131309552545

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Heteroleptic dbp-POP oxidized

Cu	5.43903067775160	3.81798015385127	3.53163980393796
P	7.50576076225030	3.24025006750971	4.35115730553598
P	3.98033361126597	4.24192086231951	5.32470685761673
O	5.59110183654492	2.09713071865787	6.33273232157887
N	4.35338239291902	2.69298316635874	2.19634377680301
N	5.36966415602311	5.23429247860646	1.94601445349102
C	3.95349802207458	1.40478969284061	2.29850620791776
C	3.09680564521391	0.83510530751943	1.31954608099310
C	2.65181722547879	1.59385534297838	0.24963884138856
C	3.07926581676400	2.93987527497678	0.11375950219952
C	2.67195636560066	3.77786856919401	-0.97721738417766
C	3.12891961205932	5.06930669085208	-1.07136054937474
C	4.03905382720830	5.59782607507311	-0.09557955655697
C	4.55463931593676	6.91805720780379	-0.17223413424191
C	5.47377524844140	7.34169296034029	0.76846770075400
C	5.89916925218107	6.46886483910547	1.80992640994371
C	4.46728746295914	4.79505481714259	1.00404272486945
C	3.95551807874933	3.44689416696533	1.12109089983762

C	4.41837680663306	0.61704005578790	3.50382945925357
C	4.36049226828218	-0.92104770300214	3.41121385097690
C	5.33789298135430	-1.53969499277952	2.39517917560525
C	5.26360135206898	-3.07323326849160	2.35482731314017
C	6.97666272430901	6.93765260768326	2.75833270553237
C	8.25829388619277	7.44039923624383	2.04444647512991
C	9.34001777392131	7.95275352276181	3.01721705057488
C	8.95964426213208	9.23620183179360	3.77156788538971
C	7.64340820515103	1.60025769719225	5.18142049139620
C	6.69827175915374	1.25880706174509	6.17484698543703
C	6.78093649941020	0.06122947592942	6.89437155261471
C	7.84844459625680	-0.81454197930494	6.63898275722179
C	8.80522169698837	-0.49599691785337	5.66128995345335
C	8.70248044303765	0.69859270861711	4.93348496470502
C	8.43360706899389	3.02686486120244	2.78785409519006
C	8.11402748688939	1.93367631881039	1.94349576894169
C	8.76356929755265	1.77971255738999	0.71242642929650
C	9.72855611711144	2.71568370558319	0.30205984907341
C	10.04143231331172	3.80821161793316	1.12870465565880
C	9.39302860277851	3.97254913636681	2.36096834647841
C	8.50952546456618	4.35823795735744	5.40685897317210
C	7.91900504807344	5.44891776104706	6.07565714935059
C	8.69163321236023	6.26702307632964	6.91501597484431
C	10.05749004482496	6.00131407201799	7.09333281526439
C	10.65099373254355	4.90741987220614	6.43996916853023
C	9.88288243534829	4.08315303704664	5.60714121111459
C	4.75444827976577	4.20252513543304	6.97428899941051
C	5.58636849324585	3.10168302038123	7.29061333344364
C	6.29545034579343	3.04169609241553	8.49625788662058
C	6.14490274471551	4.08783023225398	9.41921693994587
C	5.29516249906440	5.17442964075932	9.14553225413884
C	4.60815903732964	5.23655165137843	7.92656242571662
C	2.55752867187496	3.09653690724709	5.35153942528886
C	1.70192815280624	3.03615405248299	4.22519710252967
C	0.57662998436627	2.20151919676755	4.24265325394915
C	0.30277259850869	1.40976541409675	5.37178536339332
C	1.15321469549903	1.46094458152821	6.48847483836006
C	2.27742982390625	2.29919525311878	6.48388474799511
C	3.27788534690384	5.92676605055019	5.16306136798558
C	1.88541905175309	6.17306129385870	5.17226966658512
C	1.40596415933113	7.48901615133359	5.09908153919384
C	2.30063802867366	8.56798899919936	5.01698257113521
C	3.68652092887772	8.33080502876406	5.01170193246678
C	4.17339531908529	7.01974738469899	5.07688514100865
H	2.78474745103244	-0.20589613332242	1.42368302014425
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H	1.99349641348012	3.36715929395066	-1.73155505486305
H	2.81761165252423	5.71303954075878	-1.90007762448886
H	4.23140577849786	7.58106413352758	-0.98167089725722
H	5.89388676058788	8.34918545393886	0.71523276509287
H	6.01110666632729	-0.17997553599286	7.63315485231758
H	7.92598767452071	-1.75046274778083	7.20035488852897
H	9.63457027935690	-1.18091473700222	5.46164175698705
H	9.44275554853948	0.92920517106755	4.16186109856762
H	7.37636738597291	1.18898922719674	2.26075783651746
H	8.52319410731917	0.92307226427240	0.07527361309834
H	10.23918952892245	2.59117179511513	-0.65775569060286
H	10.80249144233529	4.53060566615188	0.81746397363815
H	9.65465502034342	4.81750417185946	3.00379798165946
H	6.84802515884333	5.64395405179537	5.96900064726807
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H	10.65969145275064	6.63994647078317	7.74694027449336
H	11.71453734520967	4.69227896402674	6.58259646867538
H	10.35552378428799	3.23142081125873	5.10783661182962
H	3.81532663754282	0.95415495296074	4.37044773739818
H	5.45561710200673	0.92340118116540	3.73472034044124
H	4.59355073750741	-1.31613605994316	4.41730350433913
H	3.32637449814871	-1.25732523287971	3.20272481094602
H	6.36804474549763	-1.22504460759425	2.65836769836345
H	5.14199459815212	-1.13341273463687	1.38333138834407

H	5.49003873254598	-3.51141616392747	3.34299332657987
H	5.98332203401137	-3.48998524964198	1.63066653856297
H	4.25672809203590	-3.41877618131242	2.06050622052893
H	7.24388334001343	6.11780612694039	3.44833421658562
H	6.56875869222988	7.76161077347258	3.37568700189618
H	8.00232140168771	8.25501447415278	1.34139610638736
H	8.66208669638530	6.61620196710495	1.42838559494643
H	6.94668748646258	2.19095543417301	8.71355083819684
H	6.68963482823668	4.04452708319100	10.36728818232564
H	5.16592101861705	5.97094821747457	9.88377902453635
H	3.95624931829325	6.08619547832957	7.70604837230013
H	9.59542585542994	7.15706082197033	3.74515466435021
H	10.25882184517854	8.13984087017055	2.43148144641390
H	1.90421166062220	3.65566137564226	3.34501329375764
H	-0.09111046748854	2.17212511316016	3.37611382689684
H	-0.57690355698638	0.75887224885400	5.38324022001138
H	0.93420279385873	0.85577570964357	7.37359382390619
H	2.92224720651863	2.34785692302435	7.36542419795778
H	8.70626421036266	10.05156330922702	3.07060572459825
H	9.79828009545991	9.58687565471143	4.39605842056014
H	8.09535805695722	9.08794772569089	4.44424996638102
H	1.17811965395979	5.34455894258864	5.25924846476867
H	0.32697900902119	7.67049481024963	5.12002017233257
H	1.92021784986559	9.59269248753124	4.96405403005320
H	4.38627502288780	9.17102258115104	4.96090679480103
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Heteroleptic dbp-POP triplet

Cu	5.38824396466374	3.81502990383208	3.43024179007096
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O	5.65102553955273	2.02205165182734	6.25715784446221
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N	5.44340394963355	5.13985030965560	1.85516380629352
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C	2.90273478916205	0.90027140595308	1.44046769986890
C	2.36666163313354	1.69770449089035	0.40198808200031
C	2.84367301767950	3.00827143237710	0.22380924416758
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C	2.97224207206826	5.12794315335649	-1.00072913977992
C	4.00371883742242	5.60520173693446	-0.12285932739048
C	4.61905774803494	6.85938879478046	-0.26397825751065
C	5.64750307027288	7.21793013210659	0.62401227655428
C	6.06488050301028	6.33576038314303	1.63766853421616
C	4.42990368702705	4.75932760057884	0.95989822768937
C	3.82896169391889	3.49673824478151	1.14569143089037
C	4.41456737377419	0.62464785806503	3.48579714273341
C	4.21636555863598	-0.90329532411643	3.45130604759960
C	5.02090781426484	-1.62898541594222	2.35732000349748
C	4.80498930086640	-3.14944145174198	2.36806343698809
C	7.23840394935452	6.73688594515213	2.50812601092644
C	8.52976955757455	7.06646749252009	1.72135642124938
C	9.66992753636136	7.59714252823816	2.61373512838402
C	9.42951364236450	9.00393556764456	3.18417474018731
C	7.72388851468638	1.76634022758888	5.03269931564119
C	6.80160921954111	1.27907300401999	5.98800307331561
C	6.93664794659256	0.01072970287416	6.56446249801863
C	8.02093475295145	-0.80128965044027	6.19542639692284
C	8.94658781958236	-0.34477744575955	5.24495349014350
C	8.79609282854201	0.92455833442755	4.66490892148247
C	8.68939896598062	3.45760597406235	2.91448890964579
C	8.21780535237910	2.93388988810132	1.68952396162553
C	9.07502384804529	2.84215310031208	0.58433778490626
C	10.40605042079474	3.27942879488686	0.68625955474360
C	10.87709389925722	3.81055376394205	1.89732519913615
C	10.02516167293109	3.90011127972030	3.01009121960441
C	8.27439382692008	4.53131224691804	5.62762865837740
C	7.70956328314685	5.78369289581251	5.94610164284547
C	8.31017820598559	6.60841719286595	6.90946599133216

C	9.47714041389609	6.19109389701004	7.56699942126259
C	10.03457813233111	4.93585908677377	7.27308792808448
C	9.43436401770292	4.10613351978552	6.31581912585535
C	4.77516522714626	4.10381307141709	6.92877306119849
C	5.66092378986168	3.03854226547164	7.20495567620614
C	6.42986142316254	3.00149325534444	8.37451962289484
C	6.29734491673750	4.04767598203765	9.29981665186080
C	5.40783368828925	5.10893595475398	9.06003919232719
C	4.65551883412950	5.14039481786813	7.87772486920491
C	2.51606872325996	2.95224834656193	5.44894154477319
C	1.59582204743386	2.89165535485557	4.37764613247497
C	0.47836446666998	2.05056521720146	4.46080986990309
C	0.27169781131346	1.26054160992750	5.60425168084440
C	1.18448472407393	1.31669464056191	6.66920147311304
C	2.30392028409603	2.15966232261707	6.59653677094445
C	3.15238934317546	5.75837776823881	5.19306876425796
C	1.88464786570432	6.01007991050194	5.76510143943859
C	1.33692633479875	7.30027571998082	5.71766024332495
C	2.04030743677409	8.34592387501160	5.09715786668349
C	3.29629935252081	8.10060160850929	4.52066562942325
C	3.84974962867862	6.81289767300960	4.56670480266701
H	2.58129865507545	-0.13710677253669	1.55167218639769
H	1.61049159262759	1.29314451055689	-0.27826355701624
H	1.66957084646223	3.50825632567839	-1.54718532466026
H	2.63743472584673	5.78210595081374	-1.81316635135039
H	4.31415075619691	7.53217011480340	-1.07216261691328
H	6.16163999940525	8.17634297495963	0.51456288262340
H	6.18279899138666	-0.33246391526494	7.27899876970106
H	8.13168225046926	-1.79379956100007	6.64286404106590
H	9.78631624123073	-0.97944264695089	4.94594245822084
H	9.51218871868038	1.26569604908082	3.91155111960628
H	7.17509817056821	2.61069970465285	1.59456099339707
H	8.69922267620191	2.43508305636017	-0.35969109246962
H	11.07354763614346	3.21072995751262	-0.17867333697915
H	11.91174198896172	4.15880147252901	1.97975870307223
H	10.40071582633491	4.32021910455311	3.94767303966806
H	6.78714465942810	6.11227445556970	5.45730227570262
H	7.85966390272396	7.57649778595002	7.14996665651457
H	9.94570186886478	6.83738202429791	8.31611015067796
H	10.93714782080746	4.59888648113455	7.79325688425478
H	9.86259845465680	3.11968039935695	6.10931248127631
H	4.00558771842074	1.02025306444774	4.43589013236908
H	5.50233578011605	0.83562798238813	3.52230781623787
H	4.52344554962789	-1.29949472579521	4.43802315226154
H	3.13994037021302	-1.14697614528813	3.36059833298113
H	6.09643112273895	-1.40464569527682	2.50083687226454
H	4.75523445561359	-1.22231488868899	1.36343676570192
H	5.09157445210080	-3.58923434360626	3.34075934957475
H	5.40451896029186	-3.64676053161257	1.58633459490003
H	3.74505967365846	-3.40558810837572	2.18866663740497
H	7.46806699625779	5.92843915934300	3.22063582471078
H	6.94738745840342	7.62056681045708	3.11120240887019
H	8.31186920348961	7.81231352670497	0.93413203987689
H	8.86011464524714	6.15013231428347	1.19924665365659
H	7.11408045271632	2.16794708487403	8.55619703293468
H	6.89095695980167	4.02663026899426	10.21911456299496
H	5.30262897760805	5.91391072408247	9.79343457663313
H	3.97478430879853	5.97362844672151	7.67992816814293
H	9.84756548884980	6.88443567708713	3.44250847867070
H	10.59975888480366	7.60685001494537	2.01470451303984
H	1.75175858570140	3.50308485105442	3.48291090818633
H	-0.23095829931707	2.01102051698592	3.62826990613065
H	-0.60200804297994	0.60380545424691	5.66573552742445
H	1.02248189193016	0.70861293765537	7.56509755314251
H	3.00423101894707	2.20828556633040	7.43544634623537
H	9.26777368402473	9.73953375272286	2.37547862011556
H	10.29688105612456	9.34498100407406	3.77529479031079
H	8.54818856867976	9.04001195882680	3.84965935932583
H	1.32889566973913	5.19802620858196	6.24349955344378
H	0.35529313238304	7.48766875668860	6.16465834930571

H 1.60540579023667 9.34971602640062 5.05675885563916
H 3.84114440627233 8.90861276761709 4.02238830424251
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(Ph3P)2Cu(N(p-FPh)2)2 reduced

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Cu 1.78456455600811 15.85855570865943 7.15575389076315
P -0.00638494304169 14.89451762964223 8.08192405344993
C 0.93314600635580 18.45101813354582 6.20513549446035
F -1.87936890369049 20.10042879664977 3.54884255505643
P 3.54239563813482 14.76397910680254 6.31260537539213
C 0.40205942053825 19.76017394043171 6.39729883496938
H 0.71152915160524 20.34089346503472 7.27092795092712
F 5.55399048148870 20.29621362860954 10.40575601423761
C -0.53410048775356 20.30771552068692 5.51240205773963
H -0.94126377188995 21.31054882790755 5.67608789982979
C -0.97163291993181 19.55951936811151 4.41340681840247
C -0.48968424020951 18.26711822052476 4.18841033719720
H -0.83697307748064 17.70194056361125 3.31794894775446
C 0.45153713588885 17.72793900982204 5.07507232243043
H 0.85449824005440 16.72358497050226 4.88599467525554
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H 2.75664558410028 16.87675190516823 9.33445865487663
C 4.12955185143823 18.44497586501701 9.91051617376982
H 4.46918372212867 17.94175321128870 10.82108807693283
C 4.63433861923903 19.70721369162542 9.58635801645211
C 4.20760105585679 20.37666611943935 8.43362016107318
H 4.63240099449522 21.35639130766182 8.19290545527051
C 3.25927259167750 19.78014429816757 7.59452596678555
H 2.95801071808590 20.29786719042112 6.67939082566015
C -1.27703512581144 16.08482116633806 8.69352422675132
C -0.83858965980326 17.34256980897430 9.15904569673992
H 0.21941522282737 17.61329287944643 9.07856266325317
C -1.76086269524283 18.25830121507694 9.68759573277022
H -1.41116587570848 19.23406974776513 10.04041971581186
C -3.12465341956950 17.93322133332709 9.74810336106234
H -3.84361736855434 18.65360843998237 10.15306053001559
C -3.56814200648611 16.68559055203076 9.27965322599389
H -4.63243564604105 16.42919553560168 9.32019322895569
C -2.65023988699076 15.76239841145190 8.75757728555368
H -3.00064684032385 14.79177293599397 8.39213057966963
C -0.99106051292578 13.76952593293697 6.99882629062555
C -1.56862155747135 14.32849152310642 5.83557597333737
H -1.45350365243107 15.40010335612047 5.63179778630676
C -2.29560893169065 13.52252705529890 4.94950752183404
H -2.74367456910843 13.96866779726657 4.05522382087652
C -2.44741195719266 12.14849550709701 5.20429213744980
H -3.01435649567821 11.51978953338973 4.50938203431772
C -1.87302469264997 11.58717898288247 6.35502035992800
H -1.99530388670233 10.51894783001837 6.56571580466499
C -1.15045821449931 12.39222892680326 7.25222195627202
H -0.71416670762915 11.94897758426385 8.15296367847049
C 0.38788836242854 13.88257709570105 9.57818435615171
C -0.31019974488952 14.02425790352521 10.79586112140409
H -1.12792691194212 14.74667106738108 10.87344866945655
C 0.04381689961185 13.24746481617962 11.90984496846592
H -0.50364434611820 13.37117943477728 12.85054361723069
C 1.09248696806924 12.31881026225497 11.82279568918588
H 1.36755061056166 11.71666010372964 12.69541553300728
C 1.79393621410397 12.17201006115291 10.61547796691620
H 2.62379586548477 11.46217040762172 10.53758368285564
C 1.45030230627997 12.95439644820040 9.50353359017411
H 2.02003422055152 12.84595651799112 8.57389040114096
C 3.10571420214564 13.65470131030761 4.89950277704441
C 2.01747936167782 12.76653136626577 5.05085656939715
H 1.45388302004254 12.74419360426192 5.99027952765191
C 1.64031048021973 11.91487788366424 4.00253315045433
H 0.79100121738507 11.23765068175217 4.13903776773901

C	2.33368402702754	11.95139796735691	2.78222347814859
H	2.03258512333456	11.29493564990170	1.95875638013799
C	3.40773106783370	12.83976282038386	2.61848530753031
H	3.94903013785940	12.87770180515304	1.66691410504142
C	3.79523922060356	13.68572507039215	3.66918457819254
H	4.63263156499858	14.37599835987503	3.53191161207177
C	4.48860252411357	13.69136348555031	7.47992239641865
C	4.59680676070452	12.29346751448646	7.33624370625450
H	4.14141958228505	11.79659618683046	6.47374148274270
C	5.29281064267057	11.53603717875586	8.29391751505914
H	5.37543011662560	10.45073844238194	8.16837017919164
C	5.09125105391861	12.16517326530486	9.39627556610887
H	6.43732006518511	11.57307047164084	10.13844253283802
C	5.79060070467940	13.55971978967396	9.54157342118075
H	6.25781427794892	14.05848356635591	10.39743031130763
C	5.09050437957179	14.31905459275587	8.59479592626468
H	5.01572281915868	15.40698983461746	8.71262373025112
C	4.85560197010411	15.85473839883761	5.61183351269315
C	6.21323392836008	15.46954241961566	5.56142123762966
H	6.52527094988286	14.51202932134032	5.99073654780095
C	7.16475585269534	16.31413089187883	4.97114171222935
H	8.21669509359768	16.00975215841262	4.94134841950227
C	6.77053136344930	17.54494762207523	4.42103487234962
H	7.51580333978069	18.20417129673311	3.96293097594834
C	5.42259924528857	17.93222397684514	4.46802886432587
H	5.11176833437870	18.89603011778711	4.05169927207098
C	4.46684205118422	17.09544715183754	5.06392295957974
H	3.42199861336893	17.41612163378742	5.13311379469700

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(Ph3P)2Cu(N(p-FPh)2)2 oxidized

N	1.80459632947532	17.80100923097065	6.97517899440296
Cu	1.90477963517701	15.88403844751978	7.18000879532452
P	0.14657588720211	14.94552161146689	8.27322389392134
C	0.91003201764966	18.28567262724367	6.01040733096848
F	-1.83406106152141	19.44979845209109	3.11474404842347
P	3.59120024790062	14.69103907967911	6.26235488076991
C	0.03309059705473	19.38290331314487	6.23843667099793
H	0.04846012485152	19.89171555925784	7.20565098054446
F	4.65165322605270	21.05691333981959	10.44806708893472
C	-0.89299228014288	19.77139219630246	5.26837365191487
H	-1.58513640532707	20.59940672517678	5.44332734396764
C	-0.94675101503870	19.06997128720191	4.05514658496243
C	-0.10653634718508	17.97573225017814	3.79858066317657
H	-0.17024835687344	17.45857463210006	2.83755209321656
C	8.0412902444180	17.58014758820097	4.77997334566621
H	1.48816990733869	16.74790334417431	4.57717983593505
C	2.47396951478319	18.67145220003178	7.82559129934695
C	3.04285915684660	18.13159242851785	9.01723434962982
H	2.89177982119900	17.06778384672680	9.23902314676206
C	3.76369323299215	18.92564047696695	9.90492925073004
H	4.18659570167765	18.51704871251155	10.82640723574383
C	3.95096440021577	20.28379018023163	9.59727271003089
C	3.44066846507105	20.84885781209947	8.41846108312658
H	3.63745247890524	21.90151311904497	8.19795064980346
C	2.70800928999180	20.05012372085123	7.53995199189124
H	2.34413632221451	20.47763384639574	6.60221497550755
C	-1.10496628776208	16.17754228840120	8.83219586639657
C	-0.65048353214130	17.33113384329730	9.50953495552094
H	0.42187772638982	17.49289370618198	9.66406017321570
C	-1.56699498682536	18.27232561091970	9.99988451672148
H	-1.20367202318181	19.15726152837281	10.53278233346169
C	-2.94516788236072	18.07991291360079	9.80811951994556
H	-3.66013592700229	18.81723431982992	10.18712438747479
C	-3.40298109823381	16.93830626258741	9.13284989674273
H	-4.47622580214221	16.78071332641508	8.98479698444703
C	-2.49069761421157	15.98655064220306	8.65068931411932
H	-2.85866237960890	15.09590301177854	8.13336424100545
C	-0.80638003396251	13.78198627549557	7.21271052701216
C	-1.31336820626392	14.27084811501717	5.98661170854719

H	-1.14706370988534	15.31622938671467	5.70022615210737
C	-2.04955879239206	13.42993228849776	5.14092009128261
H	-2.44784073496000	13.82115386864266	4.19917082241979
C	-2.27542238348809	12.09025816529807	5.50099696798116
H	-2.85160090478143	11.43428411698019	4.84046563134485
C	-1.76675808420699	11.59773840164229	6.71276352378964
H	-1.94628183382461	10.55699237851380	7.00154085623652
C	-1.03824340297263	12.43847114201041	7.57065877869979
H	-0.65720952910440	12.04982376463554	8.51967249166921
C	0.58047143443222	14.00709988415163	9.79421459343980
C	-0.05380440689410	14.24682292706039	11.03158772772320
H	-0.83047874410979	15.01258277479266	11.11124571505395
C	0.30951172759216	13.50177920035264	12.16397934221428
H	-0.18795761740019	13.69549021340216	13.11981100126736
C	1.29844734156655	12.51024256270045	12.07270992561046
H	1.57671242704351	11.93001311064596	12.95838807453570
C	1.93047069805683	12.26435107349457	10.84298174223101
H	2.70504343242818	11.49570752835393	10.76169174155584
C	1.58134922991320	13.01326511676403	9.71005734269874
H	2.08294966467927	12.81440094037974	8.75652676503021
C	3.02524741839756	13.85677310936707	4.72389628229672
C	1.93362590960039	12.96127027043521	4.79821081454249
H	1.44757131625422	12.76239805274834	5.76019095084279
C	1.47015221689194	12.31619342552303	3.64271888714983
H	0.62878300053533	11.62027607016130	3.71542950183688
C	2.07506032724127	12.57234636222451	2.40122416156107
H	1.70892825402766	12.07178025677378	1.49907785357978
C	3.14757586456538	13.47355688176028	2.31910921281177
H	3.62116995670977	13.67748354458054	1.35329968485091
C	3.62568281496796	14.11366938031818	3.47330732959169
H	4.46726845907735	14.80859521107575	3.40168971237429
C	4.35686852734481	13.38804172749936	7.31302352737200
C	4.33919788404474	12.01753639986773	6.98643497446923
H	3.86562846562746	11.67919744950657	6.05999926047550
C	4.94094988231556	11.08245382512660	7.84578094563721
H	4.92835807714382	10.02017060736913	7.58086400698002
C	5.56863435367541	11.50641347713388	9.02711783210074
H	6.04503923095659	10.77549705746680	9.68842893484253
C	5.59341438295684	12.87338988802114	9.35431287771671
H	6.08817990025568	13.21093233682941	10.27071923556565
C	4.98781701440796	13.80924439650704	8.50579142534901
H	5.02359722748189	14.87552517376976	8.75877649356376
C	5.03919384158962	15.70648526102101	5.74499233792437
C	6.33528921473312	15.14927385170668	5.66775114458532
H	6.50351358396342	14.10979496340603	5.96525273585017
C	7.41038857255984	15.92750992395727	5.21516743919327
H	8.41160118431996	15.48794323004202	5.16094131785196
C	7.20478322353775	17.26277495228932	4.83145938822215
H	8.04680813485549	17.86770117875554	4.48004023572420
C	5.91916099548708	17.82112469402835	4.90258420427398
H	5.75513531322690	18.86273115000647	4.60823612442870
C	4.84064079724784	17.04945945016890	5.36080716044369
H	3.84307697466113	17.49525972351267	5.42849739879005

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(Ph3P)2Cu(N(p-FPh)2)2 triplet

N	1.78484983971982	17.73176991282824	6.90728369934496
Cu	2.06354250714739	15.86010930127994	7.23187784569620
P	0.32797166038203	14.96876434736789	8.36583464532183
C	0.81939479247451	17.99316490140012	5.91297124777929
F	-2.08142130120227	18.45786416885971	2.96565785139733
P	3.65315363770594	14.64407823935401	6.24531832299846
C	-0.36519268122732	18.73625963642889	6.17606533130909
H	-0.53723920780424	19.13592789903889	7.17919913233015
F	3.77662225171202	21.66957307328794	10.27659700129241
C	-1.34302911827754	18.88608990388745	5.18419730632637
H	-2.27071553173631	19.43037809188323	5.38192779157860
C	-1.13557881424562	18.30812077158209	3.92736381710576
C	0.01974973127107	17.56496693324079	3.63609286454413
H	0.15149452535533	17.12967527330863	2.64212236432035

C	0.98339152188797	17.39804500354436	4.63525294510413
H	1.89505135634837	16.82857198954932	4.42381692493412
C	2.24149886670995	18.75674680242977	7.71933110734085
C	3.03562835047216	18.40246374329891	8.85041669215472
H	3.22916289577390	17.33662150104442	9.02985492428288
C	3.54952589576217	19.36978191871311	9.71192232428779
H	4.16019672597315	19.09850329453859	10.57740950122351
C	3.28602431330210	20.72236673386782	9.44070282083598
C	2.55265608373350	21.11972176797946	8.31457029676614
H	2.40346511063130	22.18520012836414	8.11817898991843
C	2.04055082431191	20.14521388099734	7.45236046639007
H	1.50221463839273	20.45015216695402	6.55193113953180
C	-0.79469300845463	16.31986702380009	8.92488897814907
C	-0.26972804400944	17.26326977474040	9.84166904270383
H	0.75233338681186	17.14452504294546	10.21766978980598
C	-1.055944490752256	18.33980538770087	10.28066317984903
H	-0.63901800621072	19.05880680706859	10.99427200289719
C	-2.37099973038704	18.49196069729803	9.81233410684526
H	-2.98385424561350	19.33226716166637	10.15627902149431
C	-2.90124178680088	17.55295585087326	8.90984222154525
H	-3.92915583230025	17.65908581586974	8.54628749973238
C	-2.12126640032754	16.46938374824365	8.47398250324989
H	-2.54614214097663	15.73752666993389	7.78084940064397
C	-0.75489112703741	13.85159509716700	7.37792981809528
C	-1.21000351901559	14.29359841179630	6.10804994309679
H	-0.97083286469253	15.30703383707032	5.76396820409373
C	-1.96872010648198	13.44638638140004	5.29003566287078
H	-2.32651808418765	13.81117370483611	4.32090806027935
C	-2.26101259124878	12.13356335589234	5.70323455869526
H	-2.84489130984812	11.46880164050798	5.05802983226025
C	-1.79070917551527	11.67981151532446	6.94977884326349
H	-2.01447290975706	10.65962756032148	7.28121277999247
C	-1.04547300366753	12.52636691067845	7.78111796762189
H	-0.68937864842425	12.16426980701628	8.75048219475305
C	0.71696902012818	14.03417185936407	9.89543439472419
C	-0.06188063378563	14.17056669109111	11.07054761834645
H	-0.91369216401702	14.85623996121349	11.08523151523244
C	0.26335656692281	13.43276464636249	12.22051784807552
H	-0.34133748309160	13.55312458041052	13.12647717067489
C	1.34585599071969	12.54141087094923	12.21152821770043
H	1.59228888325688	11.96567649837980	13.11021741738899
C	2.11211258026615	12.38626761028803	11.03898571613541
H	2.95513052555684	11.68860105816535	11.01348035985022
C	1.80698793741153	13.13428095762505	9.89503162709584
H	2.41309198186804	13.01083141949369	8.99161960602451
C	3.10280044198185	13.96505988042091	4.61929229206126
C	1.86523071135638	13.27333355218114	4.55350538906195
H	1.29586985101847	13.08069827616042	5.47070900025682
C	1.35909139872899	12.83540210688086	3.32300634870519
H	0.40709503133166	12.29399913592560	3.29860333070065
C	2.05751183543227	13.10114992260477	2.13142232890958
H	1.65459956316694	12.76876294034840	1.16889976268389
C	3.27284616005072	13.80944795846609	2.18548923637923
H	3.82397028209909	14.02294194398095	1.26255337381391
C	3.79241891063830	14.24033727153359	3.41310395464276
H	4.73865441335648	14.78978288115118	3.44288919641592
C	4.31190394722931	13.17914648416415	7.16368981171245
C	3.99155805836886	11.85137173010098	6.82103065907364
H	3.38391868463519	11.64776342102315	5.93414840509611
C	4.45334008357042	10.78641115086013	7.61649445327001
H	4.18764065820061	9.75743687331867	7.35079601657119
C	5.25795177334439	11.03889582948803	8.73859478095057
H	5.62540557887683	10.20651810833282	9.34897754714793
C	5.59930034572139	12.36115284668707	9.07218823472516
H	6.24105107989650	12.56293185612246	9.93671746108748
C	5.12135881444359	13.42789704229295	8.29437690069267
H	5.37803735563508	14.46085666225934	8.55632230545637
C	5.15482359553533	15.63110697607000	5.90305786359080
C	6.41173607463070	15.00307645405142	5.69209859665089
H	6.49641980191163	13.91475731511445	5.76844937782605

C	7.54532270427395	15.77469474886206	5.39617510458662
H	8.50913233534152	15.27757945536466	5.23774677676247
C	7.45229026404175	17.17213924434786	5.30126600587090
H	8.34108205830749	17.76948083816209	5.07204458408456
C	6.20700460977255	17.80187450522797	5.50389017397675
H	6.12380455841651	18.89182368818324	5.43471899263856
C	5.07205673899266	17.04008754119059	5.80395327712653
H	4.10984425555014	17.53556161866256	5.96968400016847

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(Ph3P)2Cu(NTol2) reduced

N	1.79287733903123	17.78903146826114	7.10213606891004
Cu	1.76599269025924	15.84040030988809	7.17968982408808
P	0.01156687040101	14.85903901966154	8.15090862182936
C	0.90965320105082	18.43305254514982	6.24165085946908
P	3.51237739797581	14.76595502579283	6.28759045670928
C	0.40632291008767	19.75566269278934	6.41316577077673
H	0.73960310632004	20.34820879961680	7.27036666397549
C	-0.53569887570359	20.29208929537304	5.53055375800421
H	-0.90368672367146	21.31117383090342	5.70954985881680
C	-1.04007760898556	19.56456075875604	4.43075322750957
C	-0.56170283248540	18.25054100144584	4.26617654127318
H	-0.92691386655169	17.64597945014728	3.42565426306994
C	0.38324080657715	17.69971785591238	5.13989616594933
H	0.75101315706228	16.67748744820693	4.96935823008544
C	2.70545389784865	18.47026558334495	7.90198649946359
C	3.19726331879856	17.82058380811320	9.06989669603653
H	2.78049347989600	16.83863910652297	9.33654779931505
C	4.16629210499933	18.40792381233668	9.89222584295513
H	4.50234320224209	17.86992619896824	10.78833845548337
C	4.70472290639218	19.67712482331669	9.60656600748183
C	4.23421108854039	20.32021785079658	8.44105037610620
C	3.26864472946585	19.74644507512700	7.60891269394791
H	2.96282732221506	20.26998887043317	6.69828071602949
C	-1.25201655671744	16.03547365667095	8.80287182205997
C	-0.81734877914895	17.30728152958208	9.23178111157561
H	0.23120938794543	17.59541795168233	9.10204928928035
C	-1.73398087616271	18.21407883976513	9.78536039814868
H	-1.38788388683259	19.20146672130140	10.10804841246277
C	-3.08760955804313	17.86540703597146	9.90812079544110
H	-3.80224921769191	18.57868357482995	10.33305390346129
C	-3.52755080291430	16.60327579696476	9.47599998152934
H	-4.58441113533710	16.32864574991352	9.56484057197850
C	-2.61546054428237	15.68956668282684	8.92802766273003
H	-2.96271399586180	14.70798087750527	8.58946669671235
C	-0.99587451660995	13.73509356328136	7.08743567741030
C	-1.60710183221719	14.29962947396311	5.94412562643809
H	-1.50224928738219	15.37326374886263	5.74500988714491
C	-2.35205525197125	13.49570233032928	5.07124310908389
H	-2.82519253704818	13.94573191018404	4.19189849130775
C	-2.48947385893959	12.11891368630556	5.31934901504547
H	-3.07041467042197	11.49197072992206	4.63441173949827
C	-1.88214735512490	11.55240503939363	6.45042947914989
H	-1.99282310241134	10.48188508200009	6.65610498840608
C	-1.14071668089126	12.35501438103592	7.33437454670752
H	-0.67799066171151	11.90766269338208	8.21981144519047
C	0.45365652817496	13.83895435412162	9.62851361767912
C	-0.20732839905020	13.97054532542423	10.86780266119753
H	-1.02571121297146	14.68855197074955	10.97421777823212
C	0.18437785495809	13.18975316687194	11.96630779054701
H	-0.33466265480278	13.30586916121170	12.92398211925499
C	1.23459969885182	12.26711672156466	11.84239738793159
H	1.53935934695105	11.66184674865088	12.70295502833586
C	1.89990585508723	12.13082237859686	10.61355545167463
H	2.73127078560727	11.42646708760124	10.50686728209732
C	1.51847123924318	12.91717569947706	9.51691206030721
H	2.06115835825519	12.81794528956829	8.57018675600651
C	3.07012110205499	13.62602563309939	4.90020972577188
C	1.98551671358973	12.73838172663333	5.07671977867375
H	1.42531867057891	12.73722504161835	6.01840730237104

C	1.60702861841199	11.86056320733084	4.05058554024587
H	0.75996992519612	11.18461952725779	4.20641378693319
C	2.29612065640079	11.86938401016097	2.82741068354182
H	1.99404923983111	11.19241487067623	2.02101206296846
C	3.36728403693274	12.75641586461764	2.63860563307960
H	3.90539824793300	12.77264843234137	1.68455970453767
C	3.7555368059856	13.62873433653008	3.66713632973632
H	4.59020197781773	14.31828890234171	3.51040220116271
C	4.51303869835698	13.72987315132443	7.44256582271850
C	4.65467854829999	12.33410274629916	7.30612216858308
H	4.19426226403271	11.81948622151048	6.45677940485056
C	5.38947046738295	11.60169038054749	8.25412467459600
H	5.49743268607905	10.51792220120542	8.13426627110288
C	5.99376047966459	12.25411062421990	9.33964472657503
H	6.56972428048458	11.68161519763418	10.07464550912430
C	5.85943932581120	13.64650852659000	9.47762296188111
H	6.32994599183759	14.16330227727431	10.32094151850404
C	5.12050191886555	14.38123458033479	8.54083721526691
H	5.01739479490298	15.46741287786376	8.65499285580560
C	4.77746702979776	15.87986351408580	5.53652049187295
C	6.14782623310547	15.54463478957135	5.47999965750739
H	6.50095400229425	14.61307381421275	5.93381449720269
C	7.05977939757322	16.40590845706518	4.85218723866246
H	8.12206949770446	16.14015534645860	4.81794025729183
C	6.61281048738042	17.60350029686417	4.27031958294139
H	7.32708859329543	18.27595113556664	3.78284461293468
C	5.25168982679877	17.94094156973653	4.32299507159743
H	4.89907219736591	18.87903573164204	3.88191164585592
C	4.33545766127185	17.08785099676096	4.95633383587742
H	3.28052349929852	17.37257018001111	5.02704424426995
C	-2.03037139888481	20.17889076155744	3.46480568566857
C	5.72343964960850	20.33335193109288	10.51362940798106
H	4.64848684893727	21.30002238282935	8.16843069262437
H	6.52939663136883	20.82340760635910	9.93685444113491
H	6.19579089875915	19.59735060817837	11.18786639340460
H	5.26899492877066	21.11524266020764	11.15378120514968
H	-2.55864824458272	19.40401019681940	2.88171894471893
H	-1.53851033897539	20.85373227327014	2.73644727263358
H	-2.79445102824518	20.78066181992328	3.99034096132778

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(Ph3P)2Cu(NTol2) oxidized

N	1.80027367626858	17.78277085398703	7.08926800274141
Cu	1.79166722110683	15.84968804282047	7.16192137014209
P	0.05876425799163	14.85448345985903	8.22929942977510
C	0.94013340216986	18.43636800709434	6.20896894702631
P	3.49974340901264	14.72820295897265	6.19090537959269
C	0.39056489044896	19.72990920515630	6.43852819027671
H	0.64185167143289	20.26709507907828	7.35690843690012
C	-0.51644528368880	20.28474517166981	5.53468431307123
H	-0.94079961124963	21.27260228593754	5.74701883006885
C	-0.91578787183526	19.60062947209438	4.36426283734219
C	-0.38687198204418	18.30660465174725	4.14949262049870
H	-0.68309945905387	17.74706351980226	3.25506606675119
C	0.50465199348513	17.72979289697029	5.05244365497341
H	0.90833108450907	16.72751232910580	4.85962797140829
C	2.65705197083207	18.49664201585168	7.92427293278761
C	3.10258839457981	17.86573841505191	9.12023031817107
H	2.71097384039325	16.87203658231392	9.37281009176605
C	3.99030200969308	18.50422855817075	9.98416351675168
H	4.29446920173383	18.00223889632883	10.90953608626492
C	4.50588001903049	19.78825067467419	9.69015110632070
C	4.09769246574911	20.39603496491910	8.48141508694790
C	3.19419836317364	19.77881239421611	7.61499386481882
H	2.93579291396286	20.25733461190393	6.66658132102238
C	-1.21358420259725	16.04523156947106	8.8290887555529
C	-0.77818558453877	17.24560831162748	9.43208366181085
H	0.29107645799316	17.47535002061755	9.48991720969654
C	-1.70968716967283	18.15071610039262	9.96030632701492
H	-1.36099845215502	19.07590922688762	10.43070343051451

C	-3.08416969488894	17.87399845299709	9.88177036065158
H	-3.81095919815481	18.58413179222522	10.28926181162553
C	-3.52406253549038	16.68487536124311	9.27994214696390
H	-4.59443783123690	16.46288020075897	9.21857619461501
C	-2.59591134989566	15.76981548464465	8.75969539484568
H	-2.94725399682467	14.84236417089590	8.29810015381583
C	-0.89466153563478	13.68096449590215	7.17999038654976
C	-1.46290964404082	14.17873684377246	5.98502105807391
H	-1.35199419285694	15.23850138990214	5.72539462542913
C	-2.19124783762205	13.32906497478502	5.14169431463811
H	-2.63573278086480	13.72556573674418	4.22304552633497
C	-2.35149977719509	11.97294351352890	5.47451764828267
H	-2.92192999395116	11.31031910260706	4.81564803727407
C	-1.78496415514851	11.47256301391469	6.65696953322588
H	-1.91530997955191	10.41918863181589	6.92602509029734
C	-1.06104096799343	12.32131703639310	7.51140587331448
H	-0.63219079918659	11.92633213600873	8.43730475327694
C	0.54477145199417	13.90904256386641	9.73121557112828
C	-0.10628814057338	14.08346091321375	10.97074053109292
H	-0.92707614041200	14.80055113686670	11.06241292279301
C	0.29820835060359	13.33828367947667	12.08898062542698
H	-0.21261326126132	13.48135632861917	13.04673997151831
C	1.34706623046438	12.41189565415475	11.98173338195473
H	1.65816852971963	11.83185824285843	12.85659338631523
C	1.99831818631726	12.23254145606021	10.75054080940455
H	2.82133665674152	11.51719996013657	10.65773062359335
C	1.60637143004627	12.98175817319846	9.63196151742502
H	2.12806199523188	12.83872409389591	8.67896033825307
C	2.98651934907389	13.64144963955616	4.79799732902400
C	1.93219427630323	12.72467606949169	5.00924071721363
H	1.43469086395250	12.67081078116830	5.98414844913454
C	1.51739901914426	11.87369666798812	3.97494524961277
H	0.70134921978514	11.16675590100419	4.15356675200232
C	2.13697545582299	11.94088820416859	2.71640491838391
H	1.80774242522944	11.28116024841187	1.90709817020345
C	3.17690165240333	12.85744602670155	2.49730583323846
H	3.66247862126786	12.91361744654732	1.51761993773993
C	3.60511404990119	13.70386232304108	3.53159910860314
H	4.41960386594865	14.41192135449443	3.35378546199631
C	4.44093651514748	13.65422527579803	7.35314186334315
C	4.57225257455950	12.26246991564110	7.17481544021859
H	4.12317647024279	11.77646180662179	6.30339856469461
C	5.28775380146965	11.49757243689014	8.11170193211156
H	5.39102960433237	10.41794947532165	7.96093200494934
C	5.88006826915092	12.11334438223463	9.22496946547694
H	6.44350498765364	11.51521840287538	9.94839390670208
C	5.75548515236702	13.50183391384250	9.40442839621574
H	6.22120908615695	13.98811963593972	10.26776486459699
C	5.03686063485433	14.26915818965323	8.47805922278695
H	4.95544005818600	15.35398983064925	8.61679896381737
C	4.79252677936645	15.82502879771394	5.46900476534961
C	6.16357589054488	15.49092972397724	5.50436458956612
H	6.49232703723098	14.57941954313832	6.01232826363624
C	7.10888816752638	16.32747599337705	4.89179334091485
H	8.17028958917595	16.06124399363475	4.92743413040863
C	6.69700377834572	17.49606411235155	4.23196708794382
H	7.43718652001226	18.14544834510141	3.75342257902561
C	5.33415858764634	17.83068944519688	4.18766943217027
H	5.00769962667051	18.74082201686724	3.67400476697232
C	4.38593401798297	17.00382516983650	4.80717611155485
H	3.32661349820120	17.27976214344200	4.77787895687807
C	-1.86416716712183	20.23308373335891	3.37510774057923
C	5.44958805678388	20.48803380379213	10.63757638381840
H	4.51230752059176	21.37309743237536	8.20863678143017
H	6.15371803832132	21.14413079138134	10.09872562931110
H	6.03458852394202	19.76911357846421	11.23532841064116
H	4.89270491624940	21.12662480467270	11.35011391790478
H	-2.41488514422139	19.47370016280680	2.79532026598761
H	-1.31557210638704	20.86346125738136	2.64901076860815
H	-2.59882872888069	20.88531240588074	3.87695717510152

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(Ph3P)2Cu(NToI2) triplet

N	1.70841651946739	17.73908362515408	7.16671956490673
Cu	1.45106450943822	15.83764913521043	7.10289610488159
P	-0.09756864664042	14.73844635256333	8.27695418472861
C	1.16326257219319	18.63041691526839	6.25511293247072
P	3.15849694442534	14.81697921096420	6.02892544182809
C	1.25432749534867	20.04925954319425	6.36147813389972
H	1.78674834456547	20.49374701403553	7.20628257606654
C	0.63407616258016	20.87193414581187	5.41748670062799
H	0.71450749070494	21.96017221929977	5.52679806217904
C	-0.10621430193592	20.34348614380213	4.33884107197905
C	-0.23124855137740	18.93503611463783	4.25783468149683
H	-0.82802552340277	18.49273247630549	3.45126742540439
C	0.37722828113710	18.10121171837118	5.19006753704388
H	0.26432445589932	17.01036839862517	5.12631533697890
C	2.70026228919176	18.16453340399146	8.07015728261873
C	2.65924730031475	17.68257747365267	9.40561673841408
H	1.81012171774532	17.06774803498277	9.72613144349181
C	3.65653020781953	18.02945807035845	10.31842140331373
H	3.58364871608349	17.66666196835766	11.35032169831477
C	4.75552003528839	18.83811939902118	9.93846444626482
C	4.80568738197273	19.28853051618817	8.60468735463512
C	3.80263720595868	18.97223357500379	7.68083708874186
H	3.89057011931904	19.29251177840875	6.63882944451762
C	-1.57476587614331	15.76784781144741	8.59925239239725
C	-1.47371059138203	17.17900487048107	8.59116001792086
H	-0.51465753464414	17.64817120650001	8.34814524160709
C	-2.58674365994432	17.97564553116448	8.88201540411906
H	-2.48928844732862	19.06652160360287	8.86718036311673
C	-3.82891938266619	17.37881317390545	9.18309956015842
H	-4.70083853848706	18.00300825320503	9.40590223297306
C	-3.94007775197692	15.97979003426283	9.19471179449304
H	-4.90117148342022	15.50823159639256	9.42983368254783
C	-2.82803187274528	15.17346773829683	8.90853660639637
H	-2.92680376178555	14.08371278218016	8.91602676531671
C	-0.80859518924032	13.21375795343574	7.50537003534017
C	-1.65675071231861	13.38361012568148	6.38845997479866
H	-1.91346902585196	14.39628924858235	6.05656270836220
C	-2.17312713303202	12.26520469218916	5.71417679188632
H	-2.84457660932309	12.40662561851896	4.86023481835416
C	-1.83138157424064	10.96897194434706	6.13748577131661
H	-2.22813488068484	10.09604886907915	5.60719297458549
C	-0.98911643516999	10.79479474177742	7.24675252281235
H	-0.72290730918499	9.78642756479470	7.58202012142838
C	-0.48916296427487	11.91311812769587	7.94006370124404
H	0.14751858324487	11.77193440054843	8.81862916154863
C	0.51030456815386	14.18384812030975	9.92886569316651
C	-0.12874976692528	14.56339553654196	11.13506423644935
H	-1.06866396664407	15.12307821290268	11.09722736131356
C	0.43194814185053	14.22286755676907	12.37240502170839
H	-0.08146256171209	14.51590033255263	13.29534563778884
C	1.64106847801942	13.50388688321753	12.43734645419265
H	2.07678395194562	13.24256171622966	13.40755139785877
C	2.29023438283134	13.13597454697281	11.24528935327134
H	3.23678485101870	12.58531591234195	11.27654407981167
C	1.74215747790533	13.48197237443519	10.00344851080727
H	2.27384763127192	13.20831016917032	9.08435225372793
C	2.73221343170082	13.71836571329364	4.62375191358590
C	1.62723596323784	12.84424445104481	4.73899231674126
H	1.03026385738418	12.83643148922430	5.65663856991080
C	1.29477798692591	11.97512810995320	3.69244558341012
H	0.44071093025857	11.30022374889820	3.80769696544420
C	2.04844020373611	11.98007767446384	2.50103901538181
H	1.78060349152391	11.30941148601124	1.67736583514915
C	3.14574242216383	12.84436290861872	2.37796878484080
H	3.74093438082345	12.84846989582432	1.45770409439393
C	3.49840688586325	13.70372736188343	3.43150443334418
H	4.3618973247476	14.36683851398168	3.32793416566395

C	4.27742987224319	13.81803550495456	7.09947044063791
C	4.57804395345524	12.46255027810379	6.82308596549411
H	4.20518781664839	12.00213497826160	5.90295650401774
C	5.35365344914359	11.71134439754744	7.71545002769268
H	5.58503221164266	10.66629713481774	7.48066257461470
C	5.84469587312902	12.29180295104164	8.90056400691702
H	6.45210921403625	11.70126799365268	9.59450069996757
C	5.54092146603425	13.63481325631698	9.18914933666736
H	5.91198323070007	14.09676192236391	10.11081086541732
C	4.75256148211199	14.38868783839014	8.30985913498732
H	4.50468209963815	15.42734318796313	8.56026123319366
C	4.26058021658294	16.09716938778272	5.28766757382289
C	5.59339520452334	16.30829056155324	5.69291700042794
H	6.03282633422612	15.67458219647900	6.46873534022668
C	6.36116810548984	17.32688897249680	5.10540038506717
H	7.39393381717340	17.48332579958697	5.43563379631374
C	5.81256414779228	18.13687613889560	4.09541463467739
H	6.41623573123545	18.92558338619950	3.63313636767499
C	4.49035012454054	17.92224929857969	3.67468073295267
H	4.05822006731835	18.53992797265344	2.87970524927438
C	3.71591457759778	16.91161104015609	4.26518032339073
H	2.68860297917687	16.74210893209404	3.92472036157687
C	-0.74850521197655	21.24138075651043	3.30744959383266
C	5.83687734658561	19.19264870358764	10.93386983648097
H	5.65919539512421	19.89333955625191	8.27574203092617
H	6.61294404622773	19.82999453532680	10.47789031976121
H	6.33553981445236	18.28911859023041	11.33206285379592
H	5.42363745575140	19.73655451836366	11.80394467073866
H	-1.78035507758239	20.92092573052826	3.07657319383361
H	-0.18779035565746	21.22411139243906	2.35284267137657
H	-0.78508402893939	22.28971525093232	3.64848129875108

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(Ph3P)2Cu(NPh2) reduced

N	1.81347290757697	17.80639964195478	7.07202307827609
Cu	1.78257569263497	15.85588023307246	7.15523136195152
P	-0.00934012458666	14.89813370227355	8.08331712587010
C	0.94383827876554	18.44435711400783	6.19357517541357
P	3.54165403975275	14.76528787196913	6.31136279443465
C	0.42309910555721	19.76084539596687	6.36155690126452
H	0.73211192011092	20.35086061614509	7.22929739053334
C	-0.50201773047499	20.29277603659627	5.45640528920645
H	-0.88533657384207	21.30641341088220	5.62597339430766
C	-0.95574784387986	19.55112632705762	4.35072386066476
C	-0.46648441905228	18.24632558440949	4.17468592665521
H	-0.79755315678305	17.64459297371299	3.31960639425141
C	0.46021649084766	17.70544155276060	5.07383275991293
H	0.85444294098711	16.69211152360958	4.91000682365937
C	2.70182425267260	18.49050806411701	7.89500502654793
C	3.16859806462271	17.83242971980592	9.07105274279223
H	2.74865913685974	16.84621575556031	9.31632262916636
C	4.11161757387775	18.41966200945139	9.92283691936909
H	4.42902544855215	17.88071606250794	10.82375365172709
C	4.63483955141287	19.69234754326712	9.64114750889026
C	4.19797762507651	20.35353942107110	8.47905280598632
H	4.60757405938590	21.33953282982865	8.22763846375777
C	3.25671443431573	19.77477604442346	7.62048432092753
H	2.96097956000991	20.30055597442911	6.70797218105498
C	-1.26560913458793	16.09609189670068	8.71013283521942
C	-0.81068749554441	17.34132380881514	9.19324433037180
H	0.25099856661145	17.59895797844231	9.12013716584116
C	-1.72160077291560	18.26285299128401	9.73114210533882
H	-1.35879360069954	19.22900653026350	10.09691807177788
C	-3.08999181234957	17.95623132006402	9.78385303285013
H	-3.79996635902355	18.68147958192315	10.19606127861552
C	-3.54967701496028	16.72121767888066	9.29798552375438
H	-4.61764246067736	16.47936249339472	9.33237330181085
C	-2.64329715772499	15.79220782928706	8.76602002773137
H	-3.00617565067864	14.83170136600016	8.38619796623602
C	-1.00627028174421	13.79650519947410	6.98744215291608

C	-1.57660523473100	14.37336704375666	5.82929034617145
H	-1.44915007873178	15.44555620992688	5.63554749914893
C	-2.30999302394578	13.58321034216168	4.93420193161707
H	-2.75185593926256	14.04273156675806	4.04358028994256
C	-2.47565959249803	12.20820477887325	5.17455107957692
H	-3.04735140106702	11.59216615944502	4.47216480868112
C	-1.90840747824216	11.62941572844687	6.32013024016381
H	-2.04128232354771	10.56023248988237	6.51947682002113
C	-1.17923914582135	12.41820186174957	7.22633124233296
H	-0.74792503898040	11.96159193333459	8.12281142731216
C	0.37131292676453	13.86198973243082	9.56731699792340
C	-0.34577032625212	13.97524505495784	10.77693938664534
H	-1.16865574024656	14.69165821459485	10.85646590485815
C	-0.00390013483385	13.17867941036524	11.88060859238650
H	-0.56616223607776	13.28053735455562	12.81521976026997
C	1.05196619750482	12.25828088119808	11.79129456563638
H	1.31778103883393	11.64083356905413	12.65609721773323
C	1.77237688542168	12.13972994695483	10.59212710317272
H	2.60809126493629	11.43689367466699	10.51291477186288
C	1.44022915592622	12.94173947651309	9.49062962906764
H	2.02454971728073	12.85502946991129	8.56778208608915
C	3.11950121487273	13.62673335078729	4.91690953439981
C	2.02543161170235	12.74668937709059	5.07263612065126
H	1.44761519320257	12.74937950193511	6.00368469365462
C	1.66015571652179	11.87178984260090	4.03938678511550
H	0.80549895364613	11.20185902262768	4.17875617854413
C	2.37218913340097	11.87595732716425	2.82934236154054
H	2.08059840652180	11.20125401585881	2.01722953590618
C	3.45284525036819	12.75551881488152	2.66091671455908
H	4.00875915734515	12.76823948482033	1.71710102705064
C	3.82778301619919	13.62493648658993	3.69682914391360
H	4.66997046154637	14.30874527447475	3.55607513940792
C	4.50164973650705	13.72147059746583	7.49389757493471
C	4.62732231074603	12.32325787559517	7.36773339101495
H	4.17911044267174	11.81034366126065	6.51087224564433
C	5.33079637882435	11.58620981057473	8.33575561538440
H	5.42688767723611	10.50049176387864	8.22384285555433
C	5.91921978295155	12.23632773443460	9.43129965877196
H	6.47074241924551	11.66020359972195	10.18201829160840
C	5.80077870049158	13.63112982753145	9.55912710621783
H	6.25942431799974	14.14606758898987	10.41007054930468
C	5.09328356935538	14.37058620191461	8.60205347891038
H	5.00309717224396	15.45870123564144	8.70784854175742
C	4.83897258627306	15.86208423419582	5.59093642133963
C	6.20350825404167	15.50084777925000	5.55454328765953
H	6.53096543274445	14.55885096226391	6.00614442966247
C	7.14216076305823	16.34974606425294	4.94986866049544
H	8.19963952052283	16.06406851120483	4.93106613340475
C	6.72803558269648	17.56094924293365	4.37171334582844
H	7.46332566587097	18.22375099331287	3.90265138166712
C	5.37307055165015	17.92443884318745	4.40485072070708
H	5.04624486968692	18.87329830560033	3.96702042433735
C	4.43006531609133	17.08345052470468	5.01476505639358
H	3.37964418481279	17.38739073295564	5.07150444696275
H	-1.67475067045828	19.98029606370836	3.64545547128595
H	5.36677976687364	20.15808636364176	10.30889965671113

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(Ph3P)2Cu(NPh2) oxidized

N	1.80207311128956	17.80483406018860	6.97285574324316
Cu	1.89992394702482	15.89468916817606	7.17976634506492
P	0.14381586772622	14.94236204672468	8.26656832789122
C	0.90895883330721	18.28859099104526	6.00375116954004
P	3.58811351277066	14.69355992412211	6.27152611988357
C	0.03294308275844	19.38456942128639	6.23235168712010
H	0.04949305253252	19.89103536042174	7.20105066289781
C	-0.88801813608316	19.76706986582019	5.25178903998330
H	-1.56708078395165	20.60252160817172	5.45010496863312
C	-0.95585261777620	19.08187312029274	4.02610811417603
C	-0.1012655653799	17.98863804559591	3.79356210471034

H	-0.14069019226597	17.45364529422199	2.83928484074751
C	0.80984835202360	17.58388399051470	4.77341585569378
H	1.49767585225315	16.75323474855073	4.57445877651361
C	2.47495445779147	18.67658977760607	7.82153814896238
C	3.03522743561409	18.13954711154657	9.01733252251666
H	2.87547672418154	17.07705717081381	9.24241386775831
C	3.75584865466613	18.94398386418857	9.89859182546528
H	4.16186302533962	18.51233297001160	10.81889234192866
C	3.96515788808388	20.30578636799731	9.60439284982350
C	3.45019957991216	20.84447148899360	8.41140117929424
H	3.63505854589119	21.89432503958484	8.16213515979984
C	2.71465090683772	20.05093877377662	7.52682865098624
H	2.35330088826797	20.47158436560895	6.58477563799557
C	-1.10541258976444	16.17119167049940	8.83602016323647
C	-0.64961768179008	17.32554424325075	9.51093885071479
H	0.42328623792733	17.49331015619165	9.65463765644191
C	-1.56609630682990	18.26220329151994	10.00990726218908
H	-1.20165535603703	19.14882832216719	10.53911413468374
C	-2.94494482233809	18.06408113561186	9.82975427654444
H	-3.65970905371520	18.79821559230762	10.21533767537910
C	-3.40392072005200	16.92161690519472	9.15659622709655
H	-4.47772271734022	16.76016210283685	9.01684816625948
C	-2.49181641074181	15.97461913888582	8.66522799212419
C	-2.85990001907598	15.08370651748031	8.14838234635547
H	-0.81040501696721	13.79375451673367	7.19147116823356
C	-1.30633468059675	14.29692348981129	5.96658817091129
H	-1.12954326031670	15.34291290587674	5.68872911434712
C	-2.04415488973248	13.46835522457824	5.11023875751172
H	-2.43289895821623	13.87002916842701	4.16891157405700
C	-2.28343820183748	12.12790087188871	5.45845196503722
H	-2.86095978635988	11.48187575994286	4.78930240853760
C	-1.78634291187449	11.62163654964931	6.66936997437342
H	-1.97645148974656	10.58027545860296	6.94908563148836
C	-1.05566827346272	12.44956403615804	7.53785011137746
H	-0.68315035261544	12.05047723934575	8.48593803660527
C	0.57358694802455	13.98670728084514	9.77760674977477
C	-0.05395740997619	14.22279074203045	11.01908642956948
H	-0.82260453391978	14.99566126557621	11.10742668456865
C	0.30584721802981	13.46508038082556	12.14415442277755
H	-0.18643400516770	13.65595132770830	13.10324809007966
C	1.28467050501980	12.46466910837934	12.04147639148702
H	1.56018300182380	11.87453270021394	12.92146770426643
C	1.91046818574395	12.22290741063270	10.80774827171260
H	2.67778307211825	11.44798008887818	10.71774084038070
C	1.56484338514963	12.98438636826533	9.68224417966374
H	2.06273025720472	12.78997167860330	8.72592311439327
C	3.03148745592858	13.83662401940366	4.74248784627446
C	1.94317019887816	12.93798080137975	4.82457443913620
H	1.45271245256884	12.75186958521462	5.78679464881066
C	1.48761381906205	12.27444852328292	3.67647975033921
H	0.64827169303204	11.57673004323772	3.75520109556942
C	2.09754199836728	12.51496483282962	2.43433190538676
H	1.73761968448606	11.99999316540856	1.53779199205783
C	3.16685268049650	13.41919810985043	2.34420091557284
H	3.64408235981343	13.61126895485752	1.37774786389311
C	3.63681642873613	14.07792025242418	3.49118071762377
H	4.47551469688185	14.77566330264069	3.41355143705437
C	4.35981709061679	13.40858902190690	7.33947867325949
C	4.35859120819597	12.03500695819677	7.02547250248197
H	3.89400209080102	11.68337112899643	6.09942665171350
C	4.96511065221758	11.11433457997171	7.89698113650991
H	4.96563323593753	10.04958446928610	7.64174881824903
C	5.58092543221592	11.55594664926120	9.07812128265804
H	6.06089743638483	10.83630001204542	9.74916597587824
C	5.58906350535675	12.92604254096774	9.39277448479145
H	6.07415556064538	13.27717073345241	10.30924165636257
C	4.97894806936564	13.84761924325209	8.53199859653753
H	5.00181846129545	14.91647516854646	8.77538469781738
C	5.03065649227869	15.71228870269708	5.74580099221647
C	6.32989308169875	15.16119489857713	5.67675364922546

H	6.50328297408880	14.12592550361986	5.98580089353051
C	7.40149254046490	15.94020862919783	5.21746434008782
H	8.40513282142716	15.50541537567883	5.16961050656368
C	7.18929497590977	17.27022784113069	4.81929643683012
H	8.02865651970948	17.87594248884998	4.46282344029461
C	5.90069147548550	17.82244727586413	4.88272224908678
H	5.73130204385153	18.86014486584884	4.57795046211306
C	4.82544073983485	17.05001231123789	5.34727452477308
H	3.82584939597692	17.49184279655350	5.40907499785291
H	-1.67313831294035	19.39272433523869	3.26048234672476
H	4.53756325550581	20.93579565491279	10.29174758991458

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(Ph3P)2Cu(NPh2) triplet

N	1.77312955570246	17.73789493781524	6.91324132050114
Cu	2.05632588946737	15.87378596572740	7.24376340015143
P	0.32185268590047	14.95723749681642	8.36502299721339
C	0.80867869695475	17.99717814633879	5.91590673894551
P	3.64719613389318	14.65113600149629	6.25885468721530
C	-0.36412469872549	18.75900812776522	6.17283616610112
H	-0.52144818358279	19.17759036573942	7.17107214257526
C	-1.33761659600191	18.90567089124579	5.17703823197260
H	-2.24617128267658	19.47667062639594	5.39744987541514
C	-1.16612155137844	18.31784326292819	3.91234820903002
C	-0.00774377792153	17.55944808976447	3.65234743217606
H	0.14078926225349	17.09760736680012	2.67076526736466
C	0.96287306529033	17.38633301640362	4.64451084939560
H	1.86834135811699	16.80432730293071	4.43858905637191
C	2.24850812414069	18.76943633180255	7.70938790059970
C	3.02107457613688	18.42325699480594	8.85654483276162
H	3.17810350221556	17.35681628890060	9.06735592351191
C	3.55875579527549	19.40522652891722	9.68627806272426
H	4.14590659309244	19.10988122131929	10.56241458504995
C	3.35933212501945	20.76960014053850	9.39483992446434
C	2.63291037899923	21.12988540471158	8.24571780538739
H	2.49975128241139	22.18768630671692	7.99351429759335
C	2.08689010516341	20.15432182437767	7.40608888868903
H	1.55418336924668	20.44751465369038	6.49786906132806
C	-0.80595834067354	16.30327787937265	8.92553612530383
C	-0.285344446731910	17.24919345607973	9.84205992344521
H	0.74110013711558	17.14237164273971	10.20957890825480
C	-1.08089909646367	18.31441250278373	10.29109139206756
H	-0.66631883519886	19.03623574026858	11.00321825802795
C	-2.40140888444477	18.45235092323140	9.83406229040932
H	-3.02154728214533	19.28400538757514	10.18593949070993
C	-2.92714414744202	17.51079126478808	8.93138216930526
H	-3.95865034422762	17.60670285118142	8.57515263660815
C	-2.13776775484147	16.43890025507380	8.48486988137473
H	-2.55837467426467	15.70493360832993	7.79140560853229
C	-0.75055055230905	13.84833862701446	7.35929279602718
C	-1.20207951274492	14.30430432509326	6.09227838578559
H	-0.97096651693287	15.32444154691380	5.76292350026030
C	-1.94837332089757	13.46123814218158	5.25896980977825
H	-2.30269500773102	13.83622079161689	4.29241112440716
C	-2.23251309541767	12.14037263397601	5.65222141454747
H	-2.80711633810969	11.47960961251196	4.99465232204639
C	-1.76542270438380	11.67356789850841	6.89579406782257
H	-1.98310994987774	10.64736931979102	7.21251643692459
C	-1.03168521802883	12.51453432777048	7.74230286174157
H	-0.67739704861574	12.14209901151548	8.70844159677983
C	0.70375390398924	14.01228004355202	9.88937158772580
C	-0.07486100594712	14.14970004608109	11.06485722557337
H	-0.92037006774387	14.84295656105962	11.08254308022551
C	0.24268212821589	13.40280502633299	12.21107933306254
H	-0.36197230971502	13.52373244161850	13.11704598494178
C	1.31689707388038	12.50160098850909	12.19845194396007
H	1.55695581456479	11.91847215536735	13.09412412033281
C	2.08299795747398	12.34589161604000	11.02558580553109
H	2.91969749768324	11.64083091082811	10.99687606149038
C	1.78582423866456	13.10264362186488	9.88537149167841

H	2.39111361045107	12.97806951276966	8.98168948947001
C	3.10721213514770	13.95805745276980	4.63661787206703
C	1.87298669192828	13.25956587037474	4.57075958752121
H	1.30253391908208	13.06740279460390	5.48728654592315
C	1.37268111195138	12.81344114402563	3.34079780386139
H	0.42338972174239	12.26721641262276	3.31684775496865
C	2.07259559430455	13.07719672707996	2.1498000115339
H	1.67399984718663	12.73816158520437	1.18774949357814
C	3.28405472694644	13.79312548555080	2.20374240312784
H	3.83667086537425	14.00517138684570	1.28131898963666
C	3.79748307359183	14.23311052073304	3.43026180213972
H	4.74004011765084	14.78884114467501	3.45987321987071
C	4.30613450064577	13.19821242741233	7.19336317124405
C	3.99963211867260	11.86590628432431	6.85637566079026
H	3.40011618490977	11.65239523134057	5.96626571965839
C	4.46340782362457	10.80980558808803	7.66276297625056
H	4.20750536464001	9.77695399875848	7.40258468428221
C	5.25773353408950	11.07684152824385	8.78934271220302
H	5.62736590036524	10.25153687287504	9.40807593422532
C	5.58639567900496	12.40364395955195	9.11636149592805
H	6.22022491934961	12.61597703758462	9.98421948894330
C	5.10616226555547	13.46182508938750	8.32768511674268
H	5.35288987080111	14.49859308478018	8.58389502790043
C	5.14572029762019	15.64212141116680	5.91570209435353
C	6.40685541096868	15.01591219676421	5.72437891466428
H	6.49578936012591	13.92950334837844	5.81944398381271
C	7.53915527161993	15.78793374239780	5.42284055104387
H	8.50623108701610	15.29249725884590	5.27941925458359
C	7.44054273483963	17.18268524805021	5.30328261826137
H	8.32825544939411	17.78008578140117	5.06978184353180
C	6.19072892917892	17.81039530913796	5.48656518578359
H	6.10279660197025	18.89855010447759	5.39833017427125
C	5.05738882660306	17.04869530266187	5.79227956655034
H	4.09226386458748	17.54289641844067	5.94382140751221
H	-1.93056356833948	18.44081506336046	3.13822750713957
H	3.78244747229403	21.54153522179523	10.04574465578519

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(Ph3P)2Cu(cbz) reduced

Cu	-1.32506908586014	-4.79736936506378	-3.43386501525959
P	-0.39258228649139	-6.35697661415869	-4.72707967624586
N	-0.30698586996511	-3.21294784881257	-3.01867422667517
C	0.26119028547511	0.37933531415756	-3.34469304451641
H	0.83998491701292	1.15160369846287	-2.82376075127785
C	-4.51346238392871	-1.80623600248886	0.58295635265291
H	-4.76299176417898	-1.05270711367786	1.33788697827091
P	-3.39476713825834	-5.00777232117240	-2.60979088628911
C	-1.24316466091045	-1.61524976746573	-4.72402769896109
H	-1.80038067494603	-2.38405022537663	-5.27441358081207
C	-1.26070330287834	-0.27928784106986	-5.14253857462455
H	-1.85408209598217	0.00138144992523	-6.02055179400131
C	-4.14230732365987	-6.67526229029068	-0.41033608978417
H	-4.28455368180568	-5.75290150796677	0.16023917515849
C	1.19223530332318	-8.78964665754576	-1.80029568940056
H	0.79575117195237	-9.37554735849064	-0.96406301941422
C	1.57538126519656	-5.74894730042844	-8.34548787075755
H	1.71058735111576	-6.27599456520503	-9.29637343681764
C	0.29655251410901	-0.95680687126090	-2.90291889246451
C	1.85169362446698	-1.27369705205634	-0.80136374370830
H	2.16836468375984	-0.22851001054826	-0.70077846009548
C	1.21284668412913	-4.39408771479662	-5.90939206408240
H	1.05767788100716	-3.86023467141101	-4.96455729061864
C	-2.85017531936184	-3.10124713344479	-0.63124912310431
H	-1.80084117961779	-3.33942769628366	-0.83411516344630
C	2.00296976855449	-3.82631089616253	-6.92068314531964
H	2.46526435438510	-2.84755267638353	-6.75628395516006
C	-4.16964298431858	-9.10909498899117	-0.51283321746878
H	-4.33221807113686	-10.07705484335590	-0.02690155770762
C	-5.66961802579138	-3.39373597797940	-5.63005660999836
H	-5.68081893451259	-2.44043972077979	-6.16911542699608

C	-4.72955571890069	-3.60145404009967	-4.61141166151008
H	-4.02113251804809	-2.80419368619391	-4.35560202682457
C	-3.77988357578008	-9.05291269418086	-1.86130965710761
H	-3.63769948604327	-9.97540407765987	-2.43440173541315
C	-3.07609358545082	-9.47854224314177	-6.93124673211319
H	-3.71862370958690	-10.19412944808505	-7.45537898132772
C	-6.57560979961406	-5.61399901677834	-5.25139691506604
H	-7.30063996639366	-6.39974936728893	-5.49086344900025
C	-1.07958190209114	-9.00436294064478	-5.61940443818474
H	-0.16778426936835	-9.35348167744666	-5.12475195467746
C	-6.59346778652411	-4.40107722106550	-5.95631068836723
H	-7.32634527979713	-4.23812931149104	-6.75371381211642
C	-3.56044400790634	-7.81339749259742	-2.48079400779657
H	-3.24218205984118	-7.77846960635853	-3.52897546672628
C	-5.22124372730545	-3.38503355704746	-1.12718053893881
H	-6.01990824030566	-3.86007822992746	-1.70674803972637
C	2.18365816028610	-4.49989041960570	-8.13883317417153
H	2.79344670594260	-4.04990366129960	-8.92982355260133
C	0.96989150735790	-1.65540607149898	-1.83033937459501
C	-5.63752037931740	-5.82717051898500	-4.22760520250225
H	-5.63820102571501	-6.77418629536885	-3.67951378359940
C	0.60709183143564	-5.65449187267212	-6.10958795815358
C	0.79143440548278	-6.32745506177844	-7.33654402467447
H	0.31738476738837	-7.29978301516812	-7.50413058182756
C	-1.90656007180666	-9.91890279390610	-6.29198072914529
H	-1.63102250486114	-10.97889969932058	-6.31991991664280
C	1.91790535949340	-3.59445152354594	-0.03069576613488
H	2.30023421617453	-4.33789453126206	0.67825554077782
C	0.56464455970760	-3.03258485338852	-1.95296555604573
C	-0.47040145084216	-1.96102934461001	-3.59424638063352
C	-2.60383644902658	-7.20307534941756	-6.21314794701298
H	-2.89339704037023	-6.14661603341089	-6.16988661512153
C	-4.70332094004365	-4.82439788109271	-3.90031564378691
C	-3.75398618823668	-6.60886051827100	-1.76459560836090
C	1.04253467802923	-4.00183351241552	-1.04458987193570
H	0.74613705688095	-5.05372568578425	-1.14297288559160
C	-1.42201692741103	-7.63660797734267	-5.57075088389709
C	-3.87324593730811	-3.73122701777806	-1.36952418601710
C	0.31065970502758	-8.08580873945391	-2.63252881867117
H	-0.76827060016513	-8.12926422158379	-2.44116006077206
C	0.80613554878111	-7.32824794866736	-3.71904978309565
C	2.19654131352628	-7.27525264194156	-3.94302346695456
H	2.59182262505704	-6.68056547122839	-4.77189146287473
C	3.07456888262713	-7.97572073119810	-3.10108817932472
H	4.15335227263030	-7.92403751206060	-3.28316470689349
C	2.32158765322420	-2.24311499368651	0.09407044045753
H	3.00851479207071	-1.95575252588378	0.89767906726944
C	-3.42179261586979	-8.11750168053100	-6.89224543610344
H	-4.33570195316045	-7.76556589209005	-7.38193173392805
C	-4.34424938558712	-7.91883287121979	0.20930078271880
H	-4.64230127750605	-7.95449620848301	1.26276105033333
C	2.57697766152487	-8.73506344362788	-2.03149787814603
H	3.26532856909261	-9.27786238856966	-1.37504990727434
C	-5.53683459127072	-2.42559395505180	-0.15504027283148
H	-6.58387732658673	-2.15806712951573	0.02475865823916
C	-3.17318676755987	-2.14509747750559	0.34461859489402
H	-2.36972856444012	-1.65605372875301	0.90459864888812
C	-0.51881453233389	0.71407978286733	-4.45916793606446
H	-0.55231513024887	1.75133459623615	-4.80993589437102

#=====END

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(Ph3P)2Cu(cbz) oxidized

Cu	-1.32295675953299	-4.71234581675605	-3.41488676645731
P	-0.45346839797974	-6.28024262577091	-4.79432335270632
N	-0.26560803378953	-3.25475576804823	-2.84186339225142
C	0.68944905512402	0.25783696677375	-2.97368229942379
H	1.31461915020088	0.94787471126077	-2.39769993873748
C	-4.83387384214522	-1.58030215901091	0.17884785334639
H	-5.15121242562800	-0.78673478352110	0.86293164200061
P	-3.45183163760836	-4.97962343895644	-2.68274314836148

C	-0.94874580589289	-1.50664329784100	-4.51464969918175
H	-1.55963117155011	-2.19055405070664	-5.11451334109419
C	-0.81090164759712	-0.15811457046366	-4.87472127257959
H	-1.33178038125080	0.22167078889869	-5.75886504308975
C	-4.00936857722717	-6.48380906283556	-0.33384809597091
H	-4.19136318617847	-5.52577665344120	0.16166877088421
C	1.38724180892353	-8.54527490321011	-1.89361410507269
H	1.06527376060825	-9.10928524535983	-1.01208667894982
C	1.00862467814959	-5.42661644192152	-8.58366994036781
H	0.94810792484616	-5.85553257643866	-9.58910947836436
C	0.56412984615161	-1.08371424209978	-2.60189936236307
H	1.98213143645758	-1.66291494346472	-0.45708502676679
H	2.40335949650229	-0.66719966298726	-0.28409625123568
C	1.15676968306945	-4.32868859152709	-6.00298576608474
H	1.21731526257316	-3.89622294049355	-4.99852703323081
C	-3.09260535730504	-3.03777937935533	-0.69099867214419
H	-2.04968257034090	-3.37222063403488	-0.68402099879945
C	1.84148235635490	-3.72094505561971	-7.06509694613959
H	2.42810822283473	-2.81490521908623	-6.88284803894408
C	-3.90080036591429	-8.91489322516284	-0.23543431036394
H	-3.99734845297026	-9.84515074620099	0.33345883937514
C	-5.61206582689422	-3.95979729140107	-6.02393768699893
H	-5.58297278670517	-3.14792524267571	-6.75776028372974
C	-4.67529212458825	-3.99103761542459	-4.98182974898302
H	-3.92957400847682	-3.19094206470719	-4.89969174832613
C	-3.55570686971474	-8.95503097673023	-1.59703420008440
H	-3.38576489344869	-9.91528778582349	-2.09473974314264
C	-3.14330649353391	-9.52781580652935	-6.76062461744132
H	-3.78145140881873	-10.27945239677113	-7.23631881657235
C	-6.62889975207921	-5.99601935503200	-5.16942263991802
H	-7.39608814597458	-6.77446479672229	-5.23422840405581
C	-1.11934393171906	-8.95404365918512	-5.53447278883243
H	-0.18225491470342	-9.26078027632697	-5.06043990782778
C	-6.58866843140722	-4.96597409465968	-6.12179457017563
H	-7.32091212834082	-4.94097876398372	-6.93514495054791
C	-3.42786591707572	-7.76429766692914	-2.32721685769163
H	-3.16352168317270	-7.80214625498457	-3.39002158053167
C	-5.35464556499528	-3.16183121767828	-1.59621214433121
H	-6.07842909683764	-3.59837077114722	-2.29106543050321
C	1.76527752668260	-4.26627235980801	-8.35701107104991
H	2.29391348001181	-3.78595448367627	-9.18660920120967
C	1.11556371357014	-1.90394601334911	-1.52696565886821
C	-5.69382516348883	-6.03113323553541	-4.12200910192931
H	-5.73453682611609	-6.83565533952260	-3.38200721559505
C	0.40202916840803	-5.50365224016652	-6.22417779060834
C	0.32975564485649	-6.04754659017489	-7.52442315878390
H	-0.25401792922799	-6.95400749110607	-7.70863997134560
C	-1.94291161062954	-9.91398080908519	-6.14349768065671
H	-1.63985421330965	-10.96606528068999	-6.14089503820655
C	1.78506588152496	-4.02315199432615	0.19612151044427
H	2.06333863772499	-4.83488621202409	0.87497963863335
C	0.58007076219743	-3.21777336491962	-1.72940819263424
C	-0.26469453477904	-1.96326416459926	-3.37223019769566
C	-2.70992238713491	-7.21215879321362	-6.15452811869000
H	-3.02094418019818	-6.16161358168272	-6.15855670745544
C	-4.70641316976570	-5.03046994114249	-4.02378562067081
C	-3.66419663501219	-6.51805815529200	-1.70073006811180
C	0.91329845366447	-4.28357083731210	-0.87229900024533
H	0.51924649342327	-5.29128454313279	-1.04479427593105
C	-1.50036603222647	-7.59515341117636	-5.53190235600336
C	-4.01766761491511	-3.61524891718992	-1.58793950788327
C	0.43430551619787	-7.88044932291173	-2.67829875248817
H	-0.62708323902241	-7.93865681932108	-2.40737485239007
C	0.83780072040537	-7.16011116547249	-3.82743169587501
C	2.20471357665310	-7.10475881237999	-4.16698940309119
H	2.52753132537319	-6.54805080151241	-5.05166641102528
C	3.15301800414328	-7.76777820998404	-3.37200688906620
H	4.21213550790342	-7.72297567845718	-3.64533892329988
C	2.31109492964327	-2.73151026566118	0.40319488706274
H	2.98935177809631	-2.55467834225423	1.24369130383270

C -3.52369970023953 -8.17565058735179 -6.76795507548394
H -4.45880585254068 -7.86737067615626 -7.24554938017342
C -4.12408204870484 -7.67999116169651 0.39216707756796
H -4.39532282473612 -7.64367700602619 1.45216503684722
C 2.74852675585627 -8.48803829158252 -2.23786163707156
H 3.49162962365294 -9.00508571637750 -1.62242875676234
C -5.75588332978719 -2.14581796578964 -0.71643855486081
H -6.79332402663472 -1.79647987173000 -0.73073523141492
C -3.50362448614673 -2.02937413465402 0.19282511799033
H -2.78009339593526 -1.58796859490654 0.88552187396092
C -0.00533047336429 0.71391825707670 -4.11340348851125
H 0.08547208352722 1.76234253036666 -4.41376948848263

#=====END

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(Ph3P)2Cu(cbz) triplet

Cu -1.35965171261510 -4.69283786016926 -3.40162284442668
P -0.48980129636032 -6.24041189805088 -4.76646924170926
N -0.25813549794282 -3.28484844325393 -2.80392195863612
C 0.89492268411826 0.17061453165798 -2.98807330104316
H 1.55762029691713 0.83234160219455 -2.41967342235449
C -4.88031475309524 -1.48479092764599 -0.01572481037760
H -5.21157292783559 -0.66278409423712 0.62757741930899
P -3.46081372755682 -5.01831105656652 -2.70083399338908
C -0.84200343503740 -1.52535769535195 -4.49961202015266
H -1.49656561465453 -2.18704074955140 -5.07841215202582
C -0.63251647407135 -0.18973161154589 -4.87573146074792
H -1.13374277740908 0.20458385983991 -5.76561294298164
C -4.08092673035883 -6.44796324554356 -0.31132250697052
H -4.31092443171585 -5.47360451851558 0.13085957701717
C 1.36507086402773 -8.58329657224086 -1.91592881536541
H 1.04236586994056 -9.18201962134668 -1.05713682843824
C 0.88475386880500 -5.23697499529607 -8.54877892476858
H 0.77748303790880 -5.61869128700695 -9.57042392732208
C 0.70065148728489 -1.16172861932724 -2.59909510478825
C 2.10410010491310 -1.79139758585682 -0.45922656092176
H 2.58628660638707 -0.81914422376038 -0.30926811044685
C 1.16087433823152 -4.26979558580789 -5.92688503923184
H 1.27370617455731 -3.88980679128817 -4.90617928735389
C -3.09634957902229 -2.90862377576825 -0.86668289170100
H -2.03853638883258 -3.18919984992590 -0.88382834075665
C 1.78925757283220 -3.60807759563316 -6.98760449032482
H 2.38718195936443 -2.71300597264100 -6.78421142919465
C -3.85773381149932 -8.86640412226444 -0.08015698990822
H -3.91109881418886 -9.76842824772138 0.53821305651076
C -5.77643948333041 -4.05170119723542 -5.97004397031219
H -5.84335849879763 -3.20029520876056 -6.65605338340176
C -4.83601409025153 -4.03742676960923 -4.92870046086963
H -4.16772752542209 -3.17666139558260 -4.80161672283665
C -3.49243946390626 -8.95592061369756 -1.43825078958373
H -3.27271320599909 -9.93184455497745 -1.88579518036768
C -3.14623210362618 -9.45680664311141 -6.83974037102142
H -3.76488916091297 -10.19729181138564 -7.35785285552100
C -6.56014946253312 -6.23084140502189 -5.22953706977304
H -7.23016100828732 -7.08997561795257 -5.34453320801897
C -1.14340827015371 -8.90139746068494 -5.56742327344123
H -0.20726626065210 -9.21244120598163 -5.09468233552925
C -6.63117694472631 -5.15672630730838 -6.12956009229007
H -7.35749339478007 -5.17405732506796 -6.94965476359937
C -3.40786707418632 -7.80245633938887 -2.22644749331243
H -3.11126896576146 -7.88097853988841 -3.27958772795588
C -5.38835231921071 -3.22472382427857 -1.64479933146903
H -6.11767000738471 -3.75060767332850 -2.26788854508454
C 1.65247149945479 -4.08291069892741 -8.30588475828982
H 2.13886996980981 -3.55837557424377 -9.13487415362577
C 1.21259159075922 -1.99620986973606 -1.52031233565908
C -5.63400433360698 -6.20854949878621 -4.17013568971717
H -5.59319459815621 -7.04147980376731 -3.46231441531791
C 0.38566077476508 -5.43672817586108 -6.16373663333179
C 0.25600532369046 -5.91003184296502 -7.49456765998178
H -0.34156695716658 -6.80370312170789 -7.69758891057685

C	-1.94522970555717	-9.84633845060608	-6.22345209224251
H	-1.62512576767964	-10.89377990521536	-6.25831245149992
C	1.76615968955845	-4.12044264945815	0.23498713020575
H	1.99517794463024	-4.93633472598824	0.92800625849749
C	0.59803961741674	-3.27958212453125	-1.69781163863313
C	-0.18173498769356	-2.00274593811117	-3.35268455914703
C	-2.74912812010041	-7.15768981484218	-6.14232226996900
H	-3.06385090104982	-6.10831634553362	-6.11825023998202
C	-4.75261751637599	-5.12079103913291	-4.02560045186623
C	-3.71508695864527	-6.52898810731880	-1.67761780293259
C	0.86966355398839	-4.34526927498312	-0.82123416972372
H	0.40483790427628	-5.32590489654675	-0.97124393267894
C	-1.54352547601768	-7.54371122366068	-5.50830097265032
C	-4.02082594598502	-3.60451853110490	-1.68234904563042
C	0.40937750513035	-7.92743967224695	-2.70175009594827
H	-0.65418460679844	-8.00829400793117	-2.44509077084030
C	0.80587379378001	-7.17278569338171	-3.83261719032122
C	2.18090344194845	-7.06225404531162	-4.13704080362362
H	2.50024362249090	-6.47628265805857	-5.00401744075471
C	3.13535404770010	-7.70458698353137	-3.33104781843027
H	4.19924489311065	-7.60960039961552	-3.57549219110482
C	2.37569035922456	-2.86117535435358	0.41511080350143
H	3.07125276081243	-2.71281632388585	1.24788607627720
C	-3.54441951980688	-8.10721210889086	-6.79550196905059
H	-4.48086028659564	-7.79084463685192	-7.26612551791964
C	-4.14914292974572	-7.60650697286873	0.47349909358614
H	-4.43848361727228	-7.52557519665063	1.52743243113312
C	2.73510719830802	-8.46761603619280	-2.22473764138386
H	3.48334754792720	-8.96782181433543	-1.60063260611161
C	-5.80514080298214	-2.17163202668940	-0.81797589732537
H	-6.86331208125145	-1.88686684176843	-0.80155358230477
C	-3.52187561001065	-1.86114332581235	-0.04289867774773
C	-2.79086533953208	-1.33215276156288	0.57773600221223
C	0.22026777267317	0.64925467136311	-4.12757128269391
H	0.36428559740429	1.68857464749120	-4.44138520950845

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[MePN]Cu(PPh3)2 reduced

Cu	1.03344008557671	9.22645410353281	6.06912241604175
P	-0.61984264213810	10.05486094164650	7.50697076721932
P	0.32409237212930	7.80587175521040	4.34216115733244
P	2.52713338630441	10.84240976978148	5.31159278648507
C	1.80309870409971	12.42953709820198	4.66291831650291
C	0.53444411970421	12.84070987081882	5.11204921190698
H	-0.01719846710014	12.19820480816403	5.80405988743972
C	-1.08465732127055	6.11297290072241	6.06620021825703
H	-0.19582472117343	6.21176139697549	6.69699349233773
C	1.46586672186309	6.47364190840308	3.71993336917402
C	0.52478323378606	7.76774065554180	8.58444792838881
C	-1.65470081031307	7.19445906064892	10.35935764371497
H	-2.49337849273100	6.97883227253449	11.03088767548963
C	4.87177651913833	13.24388770270341	7.80259916595942
H	5.00044314144406	14.31209359015543	8.01003931679462
C	4.51378007614257	10.51290797972006	7.27569575588265
H	4.36394508562590	9.44264650400142	7.10088978966791
C	-2.29726103633731	6.65834445778649	4.02747509148924
H	-2.35881416485464	7.17804297269610	3.06643171370119
N	1.51352066783612	8.01239691207570	7.64914741550239
C	-2.44084603928410	10.41240567453098	7.17264724517971
H	-2.94659592354890	10.46436514215818	8.15561459364368
C	-0.51557141454956	6.35570154508745	10.34570197524118
C	5.45124881870891	10.92812016503524	8.23390696193821
H	6.02321442073304	10.17081380218496	8.77920617062589
C	-2.63933631364757	11.76403574996261	6.46503215590352
H	-2.19731909383720	11.74967099215968	5.45271897466488
H	-2.19588719391787	12.60807636239123	7.02212365845241
H	-3.71894430182894	11.97268347923350	6.34738209350302
C	3.59770074474449	10.38278142033056	3.86327916100746
C	3.58199035084105	7.03593018423877	6.78573236493517
H	3.11784313708334	6.97119463598264	5.79764435544863

C	5.10048032267416	9.62423135696227	1.58884689977520
H	5.68505204988089	9.33562579259056	0.70866661955061
C	2.74200045104001	6.84646838942222	3.24302423354249
H	3.03952099652368	7.89819842404074	3.24944159081774
C	3.94181264213675	12.83577634627273	6.83388656690989
H	3.35780275468441	13.58916453361785	6.29805216045536
C	1.95003252199794	14.48318204584669	3.34232507198008
H	2.51082527085967	15.12267255899955	2.65183718319605
C	4.76910059604800	7.14753855729365	9.31260944441353
H	5.22490119088890	7.20446205164614	10.30887108534438
C	3.44303710394002	7.56412834147227	9.14648767645802
H	2.88415745526242	7.95279070418576	10.00371057724883
C	5.69924581039303	9.65129066905747	2.85788727267718
H	6.75584765617567	9.38558627449797	2.97317724718549
C	3.75757583018918	11.46457238297643	6.55484365392187
C	5.63265461718417	12.29374187071136	8.50112744915993
H	6.35702023884399	12.61652420283670	9.25689058968078
C	-1.14643118051397	6.79378925164948	4.83030868956996
C	-2.15750385480141	5.31483330629473	6.48973465117031
H	-2.09592007567724	4.80327894595925	7.45558051823866
C	4.95629177287511	10.03074075443890	3.98840415077569
H	5.44200703816290	10.06186149912708	4.96789813290112
C	-3.30552649862643	5.19163433885904	5.68980142765531
H	-4.14651073838070	4.57465860916655	6.02479732396146
C	3.74573646048861	9.97199062092777	1.45568527019079
H	3.26384760850409	9.95013844280520	0.47248154118478
C	0.67914023927628	14.87760370454201	3.79293419494760
H	0.24359848421393	15.82330806304472	3.45259692496621
C	-1.15396578395416	11.81081886953604	9.75038095095387
H	-1.36637930585905	10.92456875754341	10.37424224559793
H	-2.10736088862974	12.17627292443490	9.33205844240855
H	-0.76063337561082	12.60127570830427	10.41688554336053
C	-3.37191550417315	5.86441503622783	4.45965185804332
H	-4.26339804662962	5.77136861333121	3.82937053740076
C	2.80567189058276	7.52165970863299	7.87187630900361
C	5.52168860047022	6.67220326566775	8.22260344659598
H	6.55788352954337	6.34467247270756	8.35801871754406
C	2.01328989349098	4.14224916144246	3.22852532010416
H	1.72175572461256	3.08616204467255	3.22997292913071
C	-1.70102662318194	8.29981228960554	9.50323005430556
H	-2.59363828070444	8.93595611973965	9.51695939777318
C	-3.06516912100163	9.27376384299677	6.35499243626327
H	-4.14335158205413	9.46282775603993	6.19591055760738
H	-2.95230432509410	8.29820401198393	6.85403545919657
H	-2.58578508086119	9.19625854787987	5.36390753346353
C	1.11184675494934	5.10773106030412	3.70516193342587
H	0.13105171558425	4.79281655062244	4.07103514073350
C	-0.11054604515230	11.47254601046637	8.67243491807158
H	0.03543084541777	12.35223070314823	8.01498180458383
C	2.50990009101488	13.27198279751135	3.77466121426820
H	3.50090570077975	12.97626403932904	3.41735711911529
C	-0.64461636120768	8.60479995399468	8.62153492207308
C	-0.02641973864706	14.05445215788794	4.68266865250719
H	-1.01714973790282	14.35166862172759	5.04344252050710
C	-0.16636607372761	7.96013848980284	1.51155428220497
H	0.24406070233803	6.94755483683000	1.44482506255440
C	0.53786398561207	6.64488249163337	9.47213039902550
H	1.40295486899212	5.97399736886995	9.44691988041231
C	-0.23732866725441	8.60349983037850	2.76592001691531
C	1.23811230469947	11.13262270143956	9.33084606994550
H	1.59033227457581	11.99204613432351	9.93035128983536
H	2.01901684510906	10.88806258376138	8.59419518172234
H	1.12724694951302	10.26556780652613	10.00457468755560
C	-0.76225077881464	9.91221851456096	2.83014449522564
H	-0.80126007291070	10.43070139537647	3.79546553635625
C	2.99796459604842	10.34077602709059	2.58299066131611
H	1.94019083742442	10.59970231244332	2.46998202480119
C	3.27615028642455	4.52373610943081	2.75229411664382
H	3.97746994333378	3.76810247861936	2.38198790585112
C	-1.21291528543908	10.56157116762773	1.67032243069827

H	-1.61267966152591	11.57887953922954	1.73874077057634
C	3.63571462739407	5.88086022744114	2.75801798983275
H	4.61783231482735	6.19637735064423	2.39053699430477
C	4.90973170685323	6.62179278913471	6.95880647403269
H	5.46591274181309	6.24564246899099	6.09193482099313
C	-0.43843523701384	5.15750547579641	11.27049295609940
H	-0.30306877606445	5.47226047231272	12.32290529993197
H	0.40652832975131	4.49767060977885	11.01077609540196
H	-1.36565273287172	4.55655759334868	11.23541905558394
C	-1.13584584117841	9.91347882272406	0.42718094821839
H	-1.47956028188243	10.42166506197897	-0.48028745615253
C	-0.61086320780810	8.61307739517579	0.35118883472541
H	-0.54691205747350	8.10270306512934	-0.61623776636144

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[MePN]Cu(PPh3)2 oxidized

Cu	1.03539454209200	9.17587928543664	6.04682396407208
P	-0.60691380702915	10.03739609723233	7.51627146937789
P	0.24932194238872	7.78212120377170	4.32067981720158
P	2.56150065974458	10.82805238063728	5.27370210333739
C	1.79878263520156	12.38514745325485	4.61934690330913
C	0.51352755037676	12.76830820747141	5.04650440750383
H	-0.03996411002773	12.11609818887987	5.72755646456302
C	-1.22603250765061	6.08891032391033	6.00144877276020
H	-0.33257357198516	6.11281741216616	6.63344621480903
C	1.41294946342651	6.44757624584734	3.76809173639824
C	0.54758923800549	7.75127124979516	8.59292862030133
C	-1.57539683810922	7.13636692049232	10.35923292229108
H	-2.40185747581712	6.90834653815381	11.04126647176257
C	4.66449837654323	13.26323393755899	7.92231670082520
H	4.69361466204484	14.32468648651977	8.19005500634704
C	4.57388660545038	10.54739345464374	7.22999703374695
H	4.53780746930907	9.48295106307066	6.97781833369951
C	-2.40408830953327	6.75953010492200	3.97969986631728
H	-2.43849859542206	7.31304577573644	3.03674047532454
N	1.52298372981241	8.01584796397937	7.63899208244486
C	-2.42668062931572	10.42044991924857	7.23507154140667
H	-2.89415835723414	10.49708437594929	8.23506652120358
C	-0.43461230023869	6.29924529164514	10.33602458568905
C	5.46365274832974	10.99193988716978	8.21969862471578
H	6.11522726106421	10.26881361618820	8.72032333000898
C	-2.61676919994862	11.76878723448731	6.51663711464482
H	-2.23075267357704	11.72556380146943	5.48315017684483
H	-2.12437561291609	12.60898610389159	7.03589262883048
H	-3.69422545339784	12.00342836516070	6.45271274672754
C	3.65445269317702	10.37537378508603	3.84554654179020
C	3.58424170405498	7.05036280615874	6.78567920981775
H	3.11224790054146	6.96365243146238	5.80294981010210
C	5.18486885079628	9.68623476956600	1.57193415576917
H	5.78063944552809	9.42665898327204	0.69083361967514
C	2.68934716698943	6.82046777541082	3.28966559022392
H	2.97284092541415	7.87608078728740	3.24927235133226
C	3.78192934392211	12.82722986919838	6.92172560986625
H	3.13643617002014	13.55325283068130	6.42013356298268
C	1.93177702169542	14.44254435998456	3.30817315280990
H	2.49225102944511	15.09519660826143	2.63085153850329
C	4.76577429278148	7.21688108734809	9.32934296802774
H	5.23067031364367	7.30060294975570	10.31723062343135
C	3.44275870204194	7.63379022049285	9.15459864484131
H	2.88458784585435	8.06193675220978	9.99201418088412
C	5.79620323038649	9.79638190930083	2.8300606216858
H	6.87311552189219	9.62705635498032	2.93442246833284
C	3.73092007967787	11.46373925322777	6.56063231054271
C	5.51038440779654	12.35022140701305	8.57026931107601
H	6.20144415147784	12.69519655509489	9.34618095883349
C	-1.25187821575329	6.81566154200343	4.79018041431262
C	-2.33202576822895	5.31923336440102	6.39098052268759
H	-2.29568264813104	4.75599618608495	7.32901399152118
C	5.03893512350758	10.14337573269133	3.96191154785199
H	5.53670393298213	10.25243264648588	4.92951692214427

C	-3.48062044494819	5.27577262010432	5.58343258406351
H	-4.34569839957826	4.67862996754755	5.88956840096861
C	3.80532014585990	9.92215054165775	1.44766148177816
H	3.31739265815551	9.84370288456367	0.47078509911912
C	0.64534485058957	14.81066426821233	3.73652306439747
H	0.19916162840767	15.74922138772245	3.39206682601862
C	-1.02923629246935	11.84729581144792	9.72822685696241
H	-1.28619724835929	10.99443557812227	10.38135425106179
H	-1.96124694206467	12.25186443910186	9.30123948149788
H	-0.59299404858551	12.63392700271138	10.37022232583989
C	-3.51299545818349	5.99668527367840	4.37967668708169
H	-4.40287738375750	5.96195724596293	3.74255586548978
C	2.82444044672160	7.55499902734435	7.87380992885563
C	5.50021774692537	6.69789520563803	8.24693409077060
H	6.53206547571376	6.36300437734293	8.39181785445953
C	1.98371844527184	4.10846975614437	3.35573980389523
H	1.70005587050793	3.05116071835479	3.38153006855133
C	-1.66072131979185	8.25317040953624	9.51605735975554
H	-2.55942775592226	8.87641039191161	9.55886102914213
C	-3.09805455053607	9.28595501324501	6.44781825107424
H	-4.17525089590061	9.49955456168959	6.32659414098628
H	-2.99483266498434	8.30811066582181	6.94502421235714
H	-2.65661197240266	9.19462408057383	5.44104468832700
C	1.06822292332028	5.07919155540017	3.79356137497643
H	0.08373991306648	4.76630117572155	4.15079872101944
C	-0.00189052854173	11.43200460854826	8.66114370679716
H	0.18817020028966	12.28205689741574	7.97783375070743
C	2.50748078398605	13.24096714513576	3.74576914843397
H	3.51004550536318	12.96575326258991	3.40521458766734
C	-0.62224033581653	8.58146712284769	8.62857019069019
C	-0.06285270189075	13.97190829542923	4.60975993088214
H	-1.06508936417712	14.25114577907609	4.95175589285962
C	-0.13422559861173	7.96707019535693	1.49514631830626
H	0.27321060261236	6.95312101082597	1.43476765070985
C	0.60754222905166	6.61665022164435	9.45781486637638
H	1.47586794412674	5.95400074259259	9.39630151893601
C	-0.23841495877817	8.60987541569150	2.74769048371646
C	1.32901272768555	11.04199834291312	9.32617805254963
H	1.73602317672700	11.91170197093180	9.87110698152054
H	2.09200273833833	10.71962112446615	8.60018235395733
H	1.17497142149588	10.22796525360968	10.05586027420305
C	-0.761314449319071	9.91955633412221	2.80682040582451
H	-0.82871862379779	10.43647784381343	3.77085672234777
C	3.04306075327938	10.25812010642463	2.57560159438169
H	1.96832271695181	10.43910193729985	2.46894018560880
C	3.24791844503752	4.48723846761410	2.88038369086067
H	3.95686214787279	3.72732679604194	2.53587738524194
C	-1.17622494169476	10.57457133708413	1.63714947004115
H	-1.57406601759426	11.59263829145062	1.69704497621422
C	3.59597880607087	5.84729585447078	2.84432178313145
H	4.57502341964248	6.15903080399612	2.46619678662976
C	4.89874455368378	6.61430539755998	6.97738132813367
H	5.45581618588156	6.20230772199400	6.12994969991963
C	-0.35107438073435	5.08942217609946	11.24002361062428
H	-0.27345289657214	5.39405529820716	12.29996173449557
H	0.52643281582368	4.46530514810123	11.00583326672480
H	-1.25352895495294	4.45888735824611	11.15408080901064
C	-1.06722785705918	9.92911752115208	0.39497896891770
H	-1.38512692701699	10.44120354290403	-0.51898370210150
C	-0.54566462303693	8.62674646998413	0.32680367595640
H	-0.45941936061006	8.11997038865306	-0.64003525471894

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[MePN]Cu(PPh3)2 triplet

Cu	1.02662064389113	9.19160592369577	6.04796459834071
P	-0.60607599554357	10.01315185611815	7.54930912186166
P	0.20971582508644	7.81901449142932	4.31653376549582
P	2.54515738489257	10.83587980873082	5.29010982075818
C	1.75658631509335	12.35376740622288	4.61664499473037
C	0.44962508590325	12.71011994572350	5.01080231005372

H	-0.09567930318752	12.04660010600453	5.68845586531611
C	-1.37507132336112	6.20998294854199	5.98338901092426
H	-0.52692501644001	6.26223831709681	6.67312520556801
C	1.40830791479531	6.48943818769545	3.84170999193388
C	0.55992030836367	7.70750397373683	8.56090522947311
C	-1.51667791258879	7.07751303985686	10.37420141835329
H	-2.32201504941099	6.84457102999237	11.08125662336971
C	4.65708952268899	13.31816841354487	7.89564673525779
H	4.69548326959176	14.38851040144156	8.12789078190577
C	4.54736142970703	10.58369655490662	7.28566448633532
H	4.50547928138011	9.51264411478128	7.06643258048515
C	-2.41718086478911	6.77020182427346	3.85238900711927
H	-2.38407239034033	7.27058000878035	2.87955225048467
N	1.52431864385205	8.00273726163227	7.60130760076181
C	-2.43548396118846	10.40184390319901	7.30727488286807
H	-2.87967711501655	10.49444260558338	8.31700180565213
C	-0.40364851630007	6.21705824100901	10.28758632470883
C	5.39867584214292	11.04460369735534	8.30114171774873
H	6.01177121524344	10.32353138566818	8.85258509506648
C	-2.63690461861826	11.73884537910370	6.57120400062636
H	-2.27967733010240	11.67266233377966	5.52860814615232
H	-2.11975317828189	12.58373221699125	7.05832245812750
H	-3.71432009040823	11.98345921215439	6.53315241163101
C	3.65789316554554	10.36611756193061	3.87031722183394
C	3.58692937587491	7.10913209333166	6.67774482298173
H	3.11659200038626	7.09312278555141	5.69073061010618
C	5.21005461784734	9.59298687149441	1.63579341597771
H	5.81353208548671	9.29645944690352	0.77066330221016
C	2.57997099451652	6.85837754079392	3.13768129363285
H	2.74893513986748	7.90447566031243	2.86817313278638
C	3.80685727840648	12.86449747306059	6.87829047039989
H	3.18711136942688	13.58239093308325	6.33296525659436
C	1.85842440139341	14.41762988915962	3.29825520363577
H	2.41701314679060	15.08450019660339	2.63144988104259
C	4.783592549000921	7.12714233059338	9.21958764013140
H	5.25512341503088	7.15907664771751	10.20806328244260
C	3.45299332438191	7.53773680576240	9.07964066506874
H	2.89542211822673	7.91163631710343	9.94259724500701
C	5.78584703423141	9.64364024669877	2.91365364221465
H	6.84188193758896	9.38557631273386	3.05138052664601
C	3.74461837406967	11.49057396225220	6.54778732653292
C	5.46059756749789	12.41186302648477	8.61267109687314
H	6.12284716933530	12.76927336566553	9.40845147338799
C	-1.30419533636422	6.84848075582560	4.71815784405414
C	-2.52277278098006	5.48823840353733	6.35060284912263
H	-2.55794648638592	4.99828490662029	7.32980364986794
C	5.01994924964018	10.04345735952568	4.02500911582552
H	5.49286669505486	10.11365333459852	5.00839019209929
C	-3.6200048588600	5.40906319523658	5.48051679224910
H	-4.51737736593954	4.85305649312449	5.77272941137442
C	3.85721316448700	9.93754777585542	1.46900966664045
H	3.39864680615129	9.91525598426131	0.47468691162916
C	0.55358706711450	14.75387421559830	3.69204571760058
H	0.08948066216565	15.67944512984616	3.33535259197864
C	-1.01142332699953	11.85104186737820	9.75406086903819
H	-1.25780149593354	10.99640663522409	10.40972966909977
H	-1.95129130989290	12.25135795497019	9.33900096726015
H	-0.56839917446263	12.64041495591916	10.38970191514646
C	-3.56299424533958	6.05573000617003	4.22907950327908
H	-4.41369520974064	5.99688632151709	3.54116159990891
C	2.82661679772143	7.53242232339393	7.79930907693049
C	5.51752027756636	6.68683872932284	8.10348263482579
H	6.55630519236863	6.36064557906860	8.22041709722501
C	2.16715892146609	4.16657437550560	3.81417448651988
H	1.99844303331001	3.11733969396943	4.08025395605771
C	-1.61641216435906	8.22454100552894	9.56920121219952
H	-2.50195673482760	8.86090828318162	9.66033687435163
C	-3.13416037823378	9.26035551878214	6.55595398747087
H	-4.21072119063958	9.48685067064872	6.44383430955800
H	-3.03533197955002	8.29548172584341	7.07704238839986

H	-2.70761351091604	9.13485072813906	5.54627214080240
C	1.21016519868962	5.13054472323062	4.16716564783143
H	0.30282351408190	4.82201513760453	4.69421728986863
C	-0.00118831698873	11.43165284825279	8.67246575355731
H	0.17759735169180	12.27517490106399	7.97743536114925
C	2.46075353518833	13.23292837444777	3.74850128994962
H	3.47703742655471	12.98469755791204	3.42934791873076
C	-0.59965781795441	8.55631967124994	8.64278911178425
C	-0.15322253435313	13.88932278704279	4.55452754746880
H	-1.17167425521122	14.13716562960244	4.87329487742173
C	-0.11157715533920	7.96844752085127	1.48794242224556
H	0.24893212376114	6.93617293598563	1.45286047564334
C	0.62733971271835	6.54562570797697	9.37821173828429
H	1.48029266013305	5.87008283197009	9.26376660321072
C	-0.19256152845116	8.64653404589150	2.73064840964029
C	1.33939502552671	11.04988502582359	9.32076271121046
H	1.75043775139123	11.91867203144731	9.86558604064302
H	2.09337135872238	10.73642033329398	8.58186074100724
H	1.19824575230693	10.22756152049309	10.04436958785852
C	-0.64838985477853	9.98287790778738	2.75207649820051
H	-0.69199023088871	10.52535419133996	3.70308575048952
C	3.08238097591355	10.30813033711978	2.58049511609925
H	2.02443786088124	10.55637910728808	2.44740115336241
C	3.33116636583832	4.54099279257976	3.11856437655461
H	4.07379510415989	3.78535941506619	2.83975170914049
C	-1.02529928795527	10.63197972530495	1.56809287598266
H	-1.37139846017288	11.66987692594746	1.60586211695351
C	3.52924276348760	5.88745263051763	2.77849455670172
H	4.42499341677872	6.19526189930580	2.22809222220983
C	4.90937144610584	6.67942465002946	6.83409076721261
H	5.46558996944886	6.33624445597129	5.95593257274202
C	-0.30059407678367	4.97007021509550	11.13677320481013
H	0.55216303698201	5.02542591531100	11.84054921970578
H	-0.14121735923164	4.06705013556809	10.51777819107796
H	-1.21467005252812	4.81131619034162	11.73351780787520
C	-0.94027620596499	9.95101357621896	0.33498143034650
H	-1.22649520524033	10.45780584687130	-0.59298707207930
C	-0.48435991665659	8.62584813415894	0.30185176294898
H	-0.41619186442780	8.09357437915742	-0.65379096897142

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[PN]Cu(PPh3)2 reduced

Cu	5.21152395047549	5.02272054016045	13.07257157087186
P	5.80078060474931	3.38188033605251	14.64574449321132
P	6.94737544693607	6.34286044148305	12.22217648986473
P	3.75909816534615	4.20691146644405	11.45294371737571
C	9.36815688711651	4.80361901102438	17.30556681844919
H	10.19573852862357	5.15719004809355	17.93023757072481
C	4.86381835446538	3.00104059197077	17.34453074163426
H	5.83557973575797	3.37486349916988	17.67756352709694
N	4.74025399031301	6.70167026312397	14.15274773297133
C	8.76776277347012	5.92498813867065	11.96373916358706
H	9.30975634599278	6.88426213399076	11.86028396551728
C	2.49195433896583	5.64007688879512	9.30098624964863
H	3.08630865387566	5.03342576448385	8.61215783049016
C	8.25382250110958	5.62781626984901	17.07737867940772
H	8.20536122389907	6.63101096889877	17.51289616126902
C	7.24489454036490	3.89511168532422	15.68272385292753
C	9.31985480349937	5.17365777686000	13.18275259524420
H	8.80263416616025	4.20752101724883	13.31344101910368
H	9.18971104854373	5.74681125665335	14.11443795294294
H	10.39777814754077	4.96531662223267	13.04802255436658
C	6.41521566858262	3.25498037987740	8.40761612361821
H	7.43238220736503	3.55356313356454	8.13146320125548
C	5.75097146482445	7.61723238448298	14.37845790978282
C	2.60518429181082	5.97649569520172	15.09899370883257
H	3.02977038670290	4.97974886826065	15.24786296291291
C	1.61935065636865	6.61199876878069	8.78746864389054
H	1.54532037594825	6.75089669202773	7.70309750170492
C	3.16114888250537	1.53840546695898	12.11505834541237

H	4.22279423947406	1.36898442047409	11.90774737166099
C	4.58054112349930	2.89967975801326	15.96592686945602
C	3.43869717833009	7.00030340436813	14.57436293048676
C	1.83809973181392	6.25922955431469	11.56079119268313
H	1.93528803251341	6.15306379518221	12.64602627143278
C	2.85088853817199	8.28997305717258	14.42105862526692
H	3.45517579416105	9.09915887425589	13.99875122180478
C	4.52050039667157	3.42203198537528	9.94696070591813
C	2.60563230579422	5.44814174932728	10.69466575882226
C	6.33588569466000	1.73318204573006	13.98985643215824
C	6.19768453063511	0.53391822577225	14.72139751402717
H	5.74705914304798	0.55691012817208	15.71871292803433
C	7.98448581828242	9.35087273961705	14.91919198026238
H	8.83679877430874	10.00606982718067	15.12515864224797
C	8.99223575729510	5.11304749273309	10.67627228703327
H	10.07437732527698	4.94817014695785	10.51920836556012
H	8.59852431091703	5.61858315346590	9.77692323468894
H	8.51743034519602	4.11818812131579	10.74785665096862
C	5.20043578456614	8.15413413481561	10.95280181850369
H	5.30976613637299	8.88617290492255	11.77139683559791
H	4.38307196763039	7.46760755541527	11.22261960561878
H	4.90094825631477	8.70068597390230	10.03979668598750
C	6.91210224551912	1.68173417259833	12.70234828787886
H	7.00429468412790	2.60353873062108	12.11589246662698
C	5.82370255908131	3.78941130701863	9.56381573887229
H	6.37832155924647	4.50061110874175	10.18239447192046
C	1.26983491864224	6.22247444485798	15.44641173030290
H	0.66818415488226	5.40257789199843	15.85629531298773
C	1.51684626771528	8.52913695577524	14.77163548955622
H	1.10046174432305	9.53418157213772	14.63030343857390
C	0.84607848307379	7.40059751204871	9.65340010330011
H	0.16656862634305	8.15846807610353	9.24850116870793
C	7.34687849274489	0.46251470914894	12.15972629775842
H	7.78716155118113	0.44119978154466	11.15717233161259
C	2.35518988632735	0.46696581329513	12.52563119193398
H	2.79604708610346	-0.52999205832673	12.63112738569206
C	0.95780932275086	7.22038928352866	11.04056601740452
H	0.37572173608503	7.83641261791397	11.73315392643396
C	6.95647618810431	7.55840202203861	13.59223560957469
C	0.70728377284514	7.50017141637680	15.28744103227841
H	-0.33497926919163	7.69276798255434	15.56291936887401
C	3.90306462099303	2.63039913429922	18.29926814964809
H	4.14029136480901	2.72121030151758	19.36498834796114
C	5.72611458950026	8.58060773166768	15.43770871235973
H	4.83696387237189	8.63737932342590	16.07261356007232
C	2.65045143198790	2.14589761134048	17.89517148809579
H	1.90285123875940	1.85834608730477	18.64239908839292
C	8.03709577750358	8.41728678926908	13.87539844414384
H	8.94999864816865	8.35199133506078	13.27227914163809
C	7.19904217751095	5.17926365187352	16.26892044918191
H	6.33621860936063	5.82765627925460	16.08831480747041
C	4.40122943969965	1.97076280988103	7.98170380798908
H	3.83775614364408	1.26162923842519	7.36540470055055
C	7.62838732237420	8.43211045486585	10.33173491143214
H	7.28817192241769	9.05276608107313	9.48161812153491
H	8.57582110276990	7.95259869385723	10.03191025925006
H	7.83611074134823	9.11140056611428	11.17744945014352
C	0.44866779864376	1.95980629442893	12.67429494899820
H	-0.61178553205511	2.13210868673879	12.88881751025331
C	1.25027071272627	3.03382389141014	12.25245511273116
H	0.80573491395048	4.02650681583069	12.13749207463883
C	8.36134250072536	3.06887009180256	15.92381530507317
H	8.41034747010199	2.07055098049740	15.47837057830883
C	6.62651666956046	-0.68587080539774	14.17507464593124
H	6.51017851125421	-1.60939652455959	14.75302605267406
C	2.61502963224703	2.83449514116611	11.96482228541026
C	3.81091587153241	2.50782333752416	9.13515310676788
H	2.79370027286794	2.21257145947624	9.40957634865760
C	2.36110042602235	2.03631403870980	16.52568792686600
H	1.38803226292443	1.66058081455860	16.19231721912130

C	6.81101665569382	9.41903528664116	15.69497007618075
H	6.74550818598137	10.13225424918758	16.52588401743970
C	3.31422401100584	2.41547110052291	15.56963678733911
H	3.07155401514743	2.33202608676434	14.50712590669134
C	9.41830393993035	3.52524355920229	16.72793995005142
H	10.28340384347900	2.87609340293635	16.90360110763107
C	6.53195963285965	7.42188835897384	10.70929577950800
H	6.38777980164616	6.70774823121173	9.87467007341585
C	5.70607209612228	2.34067928194026	7.61512293126976
H	6.16521559381592	1.91867450354496	6.71458381877620
C	7.20264390435465	-0.72497200906072	12.89484177939148
H	7.53407865915973	-1.67859549743992	12.46982904153225
C	0.99451186165818	0.67383848285109	12.80827846373589
H	0.36441394927304	-0.16263384683651	13.12925732911529

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[PN]Cu(PPh3)2 oxidized

Cu	5.19634137208624	4.99584198587009	13.12928566274633
P	5.89927327940405	3.36785880621967	14.67674035962779
P	6.90473758939284	6.37565240052407	12.24957235982795
P	3.71714678313982	4.15223707337797	11.46874405242968
C	9.60768053170605	4.68387751801752	17.18814156404129
H	10.46862465109183	5.00376057587121	17.78402210757422
C	4.96601112900840	3.11027513958069	17.38460984372866
H	5.94318995742235	3.48093198705351	17.70466518042735
N	4.69915593168459	6.66970989227721	14.16451839896630
C	8.72294807174839	6.00843365208469	11.94079957642723
H	9.23549357963326	6.98493228054845	11.85116103410017
C	2.71304003127091	5.66903882611340	9.25715240974864
H	3.36197504745648	5.06196976445661	8.62013851661428
C	8.48317374991813	5.51731905919310	17.06948551233285
H	8.46089862594511	6.48967737099000	17.57196937751431
C	7.38915663700808	3.85464243099188	15.65181152532705
C	9.32170445598214	5.22619510954843	13.11842545737966
H	8.83258887596909	4.24255393245045	13.22033601196260
H	9.21076025666611	5.75374493452534	14.07927374177856
H	10.39850551626745	5.05138826602867	12.94355224420214
C	6.43799137359308	3.20145395745539	8.49100528368258
H	7.43479627348542	3.54561419541764	8.19561485839140
C	5.69868967785590	7.59800252644633	14.43268173941964
C	2.54865851990107	5.93130072590731	15.01866632841772
H	2.96988433179737	4.93150508673606	15.15640881942462
C	1.92038676231638	6.67296239794088	8.67884002187904
H	1.96399305387146	6.83751981626096	7.59707487499381
C	3.02603842668654	1.55887871037248	12.27448907046557
H	4.10360483742124	1.37555041445695	12.20346283878079
C	4.67742797679188	2.95966981105770	16.01157563816031
C	3.38606409365078	6.97384660189144	14.53843408757345
C	1.82162716468514	6.24142426417083	11.44746740139423
H	1.78240597400955	6.08797657254913	12.53036193514746
C	2.82879031326934	8.27745341820833	14.39304589436125
H	3.44571922923751	9.08057402851381	13.98009825877862
C	4.53424149296557	3.32830174093975	10.02287825946724
C	2.66957091172527	5.44016774136997	10.64897988842610
C	6.34521266496432	1.72054188619576	13.98112543092744
C	6.23960001472904	0.53389948819013	14.73925534002628
H	5.85527791447775	0.57370076736021	15.76339879260251
C	7.88366562318333	9.29686456595781	15.06982432919207
H	8.72587980221033	9.95298040627839	15.30978963551843
C	8.92643167257976	5.24068713290145	10.62151460580648
H	10.00742643818776	5.13128483451041	10.42300017196546
H	8.47879865906087	5.74917078878090	9.75022063722556
H	8.50168573018556	4.22384967619593	10.68585745530539
C	5.07100601254063	8.20479829427446	11.09631456844436
H	5.21123329966748	8.95663995451316	11.89234502048160
H	4.27116592689360	7.51403373274231	11.40571581196988
H	4.72250805916108	8.73255819744252	10.19136396920282
C	6.83571375836517	1.65129299258215	12.65942349718904
H	6.90125978016805	2.56130559324223	12.05193696585197
C	5.81512212954775	3.75456814763009	9.62095156169592

H	6.32662498833100	4.53068814394917	10.19706084474975
C	1.22034391753744	6.18911677618110	15.36885993352290
H	0.60273440046498	5.37672303564532	15.76468316349764
C	1.49181961530506	8.51770908809726	14.72311003165057
H	1.07610086001410	9.52162053318119	14.58787922185173
C	1.07082611064933	7.45498467633342	9.47612078430879
H	0.45026142452625	8.23320155685134	9.02019980617138
C	7.21908936038881	0.41958049790288	12.10619108000558
H	7.59146764583754	0.37963132698738	11.07760870046980
C	2.16804512072159	0.51432235761184	12.64861029650931
H	2.58460269001929	-0.47445717725506	12.86650675921132
C	1.02187086217371	7.23427567722111	10.86150977545861
H	0.36529332279054	7.83903711341943	11.49509242637026
C	6.90800045710111	7.55056953065658	13.65884705640449
C	0.68087131908236	7.48053913462529	15.22028533312633
H	-0.36210240600338	7.67707961497909	15.48738045187340
C	4.00355066193572	2.77887365474139	18.35221321104689
H	4.24402660683337	2.90084280531862	19.41349758971615
C	5.62613520622460	8.51283347206430	15.52679149736599
H	4.73017718439756	8.52329128906162	16.15308798530256
C	2.74802324298900	2.28640525678112	17.96674377686310
H	2.00267882273332	2.02505210656328	18.72493914073866
C	7.97533292873048	8.40073363208805	13.99214833817070
H	8.89820869584275	8.37228188143439	13.40475439169912
C	7.38277827415983	5.10952199876875	16.30106948036844
H	6.50786570850647	5.76223545761443	16.22022818269843
C	4.50114251911774	1.78396447167087	8.12982775551379
H	3.97994516358731	1.01702671449088	7.54757274215179
C	7.47429271561042	8.50352404336487	10.38246616044998
H	7.09462778631966	9.12560186686108	9.55179816140996
H	8.40972829219723	8.03270365484854	10.03917405143903
H	7.71272982677630	9.18294702320192	11.21995860716845
C	0.26528050042028	2.00796632174452	12.45519101510109
H	-0.81324806054668	2.18786313676228	12.51558523757331
C	1.11896854797513	3.05438620299719	12.06697340075451
H	0.69396854844039	4.03028747006406	11.81641776115837
C	8.51702579183563	3.01926797366257	15.78360850275529
H	8.53660123119128	2.04299268636048	15.29043482948533
C	6.62008849107851	-0.69608621952101	14.18153851150807
H	6.53330848388012	-1.61091549149644	14.77698359721465
C	2.50836463745344	2.84068251680639	11.97521743639366
C	3.87729794535184	2.33963760698582	9.25684112195378
H	2.87703638181212	2.00146818996935	9.54172042307405
C	2.45601036025604	2.12516176686040	16.60256073844626
H	1.48459952132907	1.73101033067404	16.28656731330539
C	6.70420256430700	9.34256202212358	15.83623662352052
H	6.63103964348847	10.02360918173055	16.69038253290888
C	3.40978464626944	2.46434426181587	15.63196492327657
H	3.17048178737010	2.32556881522628	14.57351005231098
C	9.62082860183343	3.43677017961608	16.54439914983601
H	10.49164533542848	2.77959625907581	16.63824345589291
C	6.39524530203595	7.48538714369241	10.79032885682105
H	6.21989125376710	6.77831177443702	9.95661594651636
C	5.78289931944691	2.20994132916453	7.74500657788925
H	6.26609412573498	1.77423669246632	6.86451751356946
C	7.11077886608252	-0.75558750870128	12.86650156296609
H	7.40443502758508	-1.71759914898919	12.43412163205998
C	0.78412945144549	0.73701765651336	12.74455058308954
H	0.11398439783898	-0.07877183951835	13.03443603440759

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[PN]Cu(PPh3)2 triplet

Cu	5.21422707920941	4.98596443957573	13.11524308084180
P	5.95405383898334	3.36340621418607	14.62780261557897
P	6.90585287173513	6.38729868324987	12.26421869927367
P	3.69210880444612	4.18747231883939	11.46440673499146
C	9.67406182796856	4.62281058646647	17.18277043971520
H	10.54338509481641	4.93215573179615	17.77270932950160
C	4.80872020019279	3.44163808419689	17.27322927846321
H	5.69912357020286	3.99181766868584	17.58900317549476

N	4.69664918875844	6.63321644319279	14.17087735966768
C	8.72919538363290	6.02773864742073	11.95436473462696
H	9.23837429786901	7.00772065526395	11.87832742252996
C	2.60524660909444	5.63023892074625	9.23230792932068
H	3.21876273620251	4.98514688325276	8.59665498754659
C	8.57865463105263	5.49037776790547	17.02390079172088
H	8.58626298446204	6.48336155942952	17.48613482749286
C	7.42592958340909	3.81711777376918	15.65550410538869
C	9.32912701729073	5.23988901635418	13.12699790988353
H	8.84305788712521	4.25440005581215	13.22512383063577
H	9.21043372332326	5.76340177867348	14.08884088445718
H	10.40811882520051	5.07007529187675	12.95446121899151
C	6.45345786360272	3.20666628688762	8.53656795053793
H	7.45751220848182	3.54232390272233	8.25466325951570
C	5.68823941941781	7.56322969238017	14.46455084883753
C	2.54917360028022	5.84023033060531	14.98275077699891
H	2.97479335544263	4.83696672231529	15.07137946962549
C	1.83087263568244	6.64221536980655	8.64869780655363
H	1.84516530533263	6.77153029469789	7.56052399842120
C	3.02971316478615	1.56767146678714	12.20247112320655
H	4.08914981009443	1.36659387689021	12.01420439823248
C	4.68654776403760	2.99740719929037	15.93970487292271
C	3.37967945017012	6.90916963687978	14.54848296689780
C	1.80579035518621	6.29717933750117	11.43097401688868
H	1.80029526797026	6.18196756737343	12.51895447657671
C	2.80897387890417	8.21034175512212	14.44607036366575
H	3.42314927672963	9.03074695113204	14.06444029116762
C	4.52013469319476	3.37366823721951	10.03310453536985
C	2.59343101262830	5.42975168418391	10.63216509608496
C	6.37763767338235	1.72044425154663	13.93992266055229
C	6.29287507977770	0.53453976347500	14.71745643701694
H	5.94091645279239	0.58654776459902	15.75231872421857
C	7.86493782104318	9.25614939051617	15.13758046235778
H	8.70538901527411	9.91111826482699	15.39259095889838
C	8.94268311459387	5.27347891788883	10.62927432385238
H	10.02546835572115	5.15265223045190	10.44213074685869
H	8.51005711278638	5.79683597089050	9.75902777107805
H	8.50375030087848	4.26156484675877	10.67437811733441
C	5.07509396505004	8.17696513815385	11.05531018691970
H	5.17676615617725	8.91536551324284	11.87007924524575
H	4.28072216438303	7.46568563959107	11.33060300789931
H	4.74046381437063	8.71373766113592	10.14947331115279
C	6.83279070250858	1.62610058702218	12.60400147025094
H	6.87963730488914	2.52795304714495	11.98257192918228
C	5.81625686524019	3.77419111906435	9.64849144104908
H	6.32659814646283	4.54788849657601	10.22980941050223
C	1.21640150320287	6.07479084999837	15.34236977154333
H	0.60562909734224	5.23895452559804	15.69834268855218
C	1.46872675352597	8.42747370187263	14.78445726152550
H	1.04304111066892	9.43154807107974	14.68116123586767
C	1.03399729797385	7.48307739633626	9.44799217611947
H	0.43324222326163	8.27559677113202	8.98898555980184
C	7.19639456465941	0.39070233298685	12.05477041586313
H	7.54153427462556	0.34145387752349	11.01685502987035
C	2.18241558254432	0.52491507449523	12.62065515312524
H	2.59423468562173	-0.48154131725854	12.75373538965591
C	1.02659422588588	7.30293242545309	10.84007497911829
H	0.42042751857225	7.95439146507633	11.47915112018148
C	6.89657433329199	7.53798022812533	13.67352403575544
C	0.66707065549043	7.36498606781586	15.24545357947266
H	-0.37846539387963	7.54228220977925	15.51853020362149
C	3.79709752110474	3.17377756369028	18.20921721097709
H	3.90886635076225	3.53101692939421	19.23892045815270
C	5.61137364011385	8.44117609144362	15.58075275139191
H	4.71752396717555	8.41962966464700	16.21002432316988
C	2.65406937325816	2.44902222150373	17.83419132084954
H	1.86880161786371	2.23824075700910	18.56844195882714
C	7.96656370249804	8.39429106079470	14.03710238860936
H	8.88974159442328	8.38928277356330	13.44926788305936
C	7.47030144146852	5.09687056633370	16.26125734364548

H	6.63398965690706	5.79104830636911	16.13281333633111
C	4.50725278754395	1.80458562189834	8.15218180400238
H	3.98860740426947	1.03508576817832	7.56901066426842
C	7.48833930054910	8.53381531768665	10.41539955808271
H	7.12028027547968	9.16572019251002	9.58559231574435
H	8.44224562596714	8.08600856260743	10.09033850673707
H	7.69219254948320	9.19840661151140	11.27414649914813
C	0.30594001382680	2.06643765645204	12.67864395901393
H	-0.75563243489034	2.26702116809752	12.86014145821935
C	1.14254626385987	3.10684461674271	12.23920605133755
H	0.72064821523471	4.10107484230650	12.06597505219450
C	8.53426323642754	2.95463555382746	15.81666920140522
H	8.52539992344816	1.96579187269277	15.34823992106060
C	6.64654681566750	-0.70318064114473	14.15713676401890
H	6.56816028010978	-1.61151864751163	14.76564973319881
C	2.51162278474591	2.87359494636587	12.00735410202127
C	3.86513849870573	2.37742510969431	9.26104191711296
H	2.85480173390180	2.05701879112203	9.52964519878425
C	2.53111297501888	1.99069676416322	16.51316322004172
H	1.65139906922333	1.41665592008985	16.20290046417403
C	6.68855343945703	9.28040581445489	15.91438667668190
H	6.61440805452871	9.93686837211425	16.78713977991100
C	3.53596018962478	2.26313422360111	15.57245564853413
H	3.42493104136853	1.90276276533026	14.54573966794024
C	9.64545885162085	3.35728548548861	16.57149105816767
H	10.49375077822675	2.67319681725304	16.68746673491147
C	6.42130448349109	7.48768306302406	10.78099687681293
H	6.28570724410827	6.78208918507915	9.93810320927390
C	5.80010485314108	2.20897179171607	7.78482207942682
H	6.29612171782479	1.75553538286130	6.92001661274216
C	7.09860494619542	-0.78479991616053	12.83117904262672
H	7.36945099537541	-1.75408316533206	12.39932824984602
C	0.82418312789426	0.77127002106581	12.86824565051529
H	0.16709835295961	-0.04247691792223	13.19473893495974

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[PN]Cu(PMe3)2 reduced

Cu	5.28815859149529	4.94763244700556	12.99869085469600
P	5.90627088322989	3.52656428354907	14.67139954172189
P	6.93676929947729	6.26702061935339	12.12722266912493
P	3.79874219800236	4.06973593896570	11.56734272326901
N	4.80501125899576	6.63334133285642	14.07685506839616
C	8.69888301013905	5.74488231302052	11.73669288634174
H	9.30816255634335	6.65253423519607	11.56307078992293
C	7.01466026093609	4.28696484819027	15.94466290017649
C	9.29976210937955	4.97026935109087	12.91914946866411
H	8.69439021241610	4.07224898527542	13.14053765056390
H	9.33633328424969	5.58968061273926	13.83071143734975
H	10.32758063587533	4.63737489467697	12.68326029779274
C	5.87104481421007	7.46009345812579	14.38378171023040
C	2.52739114730351	5.93463256814124	14.56553043635479
H	2.85904908605022	4.89625683955367	14.45247299864617
C	4.51665243136198	2.95927986094345	15.76497954633852
C	3.50050377159095	6.96724239160355	14.42361935977980
C	3.01998399664331	8.30502323389790	14.56156507256708
H	3.71629961244593	9.13726987957898	14.42102006747742
C	4.51132516753572	3.43378637591727	9.97699954057045
C	2.39968807934386	5.12840125636080	10.97358036941064
C	6.75783266267903	1.90897159636488	14.33445850835615
C	8.20916314311262	9.02117288207118	14.99415966658140
H	9.09741579672722	9.61732958050742	15.22623247014836
C	8.70089163377517	4.89355184153876	10.45356028812072
H	9.72432929064566	4.54478291195792	10.22203811971585
H	8.33364407995956	5.45522342569160	9.57715885810376
H	8.05876559344702	4.00168146303599	10.57642453544467
C	5.17383459096047	8.13948260029501	10.99571535064346
H	5.32665919472240	8.85404213581490	11.82265839887055
H	4.37102610762166	7.45147642155764	11.30716639425378
H	4.83067648214433	8.70761460546749	10.11128730638735
C	1.18436537007960	6.21229349426638	14.84871614549278

H	0.47842033700732	5.38009588919955	14.96180299505813
C	1.67521461059932	8.57385277644850	14.83949337295610
H	1.35152159138743	9.61838603505281	14.92613907263767
C	7.05347900509528	7.40326835239410	13.55879876993652
C	0.73863336613868	7.53662935967458	14.99507598225804
H	-0.31074242760295	7.75531809633473	15.21751265270130
C	5.93118214664813	8.31521206707071	15.52788978773345
H	5.06752929573851	8.35588597596286	16.19863976712959
C	8.18426403076667	8.18317319955187	13.87025040218058
H	9.06912240789979	8.12877620697591	13.22421883694833
C	7.58418712945304	8.40389905232637	10.28400537037288
H	7.22445356355773	9.06651619365647	9.47447149350363
H	8.50420308273736	7.91222100085894	9.92364797987010
H	7.84798113982718	9.04262764391260	11.14579858286206
C	2.86350570215331	2.57021631126025	12.13951602997920
C	7.06860128671759	9.07101875655993	15.81860155016532
H	7.07130054451941	9.70370306470644	16.71454324487552
C	6.48571420440969	7.40139130373370	10.67394365531275
H	6.30232729931746	6.70766803995531	9.82874218553492
H	5.05024716098359	4.25046990719850	9.46842950799350
H	3.73725124119619	3.03184875415370	9.29848183541034
H	5.23968888368720	2.63642535271787	10.20308331652579
H	2.79757706018212	5.99019726668831	10.41304640013605
H	1.85920953129500	5.51547011092796	11.85376913869576
H	1.70195427098481	4.56955282484778	10.32402402052458
H	3.57574993073553	1.78930338226870	12.45650156430435
H	2.20920249785570	2.15808414311668	11.35009216092519
H	2.23928773759340	2.84238475995245	13.00740397814673
H	7.69785301907428	2.09049947331764	13.78737841726501
H	6.11063688588826	1.28260204350259	13.69674085113152
H	6.98782518614768	1.35425725967285	15.26217157168110
H	6.56012558923695	5.23161373860655	16.28610316822810
H	7.99134236737445	4.52866315486249	15.49753031411295
H	7.1660097936368	3.61760759950852	16.81057312017958
H	4.00494571018148	3.84474521196704	16.17684162708738
H	4.88309036313208	2.33497330159021	16.59984890482361
H	3.78345691581655	2.37842370485321	15.18056693929860

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[PN]Cu(PMe3)2 oxidized

Cu	5.28195256213081	4.98737800588813	13.12287579496111
P	5.96487187121009	3.38982287870281	14.63335435396571
P	6.95770894746784	6.27727360193402	12.20224549687742
P	3.73572498510233	4.12684321498335	11.65701684090442
N	4.81173244749023	6.68312973647351	14.12658154335028
C	8.71899826301147	5.74702172487372	11.85374254299628
H	9.31118153493089	6.65284992012692	11.62452068506734
C	7.09425632699419	3.97303823858307	15.97573626572412
C	9.33158946359538	5.04951854119051	13.07773837277750
H	8.76391769309979	4.13625973728789	13.32872630380972
H	9.34206615825986	5.70266614464041	13.96638229632334
H	10.37217403011282	4.74909410969301	12.86223284476822
C	5.85298139619251	7.57242350687144	14.38565314992464
C	2.56512307045751	6.02807849284769	14.74949340013432
H	2.92699800178083	4.99820950749893	14.83349309167990
C	4.58671721538948	2.67836972883669	15.64754609789140
C	3.50008656299976	7.04985771660554	14.41705904109116
C	3.02245540622129	8.39079396642611	14.32398432645588
H	3.71057331816050	9.18446833796915	14.01978277163684
C	4.48384498870692	3.59302955103261	10.05117560073615
C	2.30390535731067	5.16647922221080	11.11834850428771
C	6.79303464435080	1.86012475105263	14.00352121470780
C	8.11180584945479	9.19112396172370	14.96320912221599
H	8.98106075657770	9.81819069400210	15.18306636326221
C	8.72331668244024	4.82339646985771	10.61981763104933
H	9.75068958478708	4.47725421610783	10.41026515283074
H	8.35220377315230	5.32771135299054	9.71157014384849
H	8.09683787115501	3.92930723919528	10.79386259169569
C	5.16730854926351	8.08665938608912	10.97734823513797
H	5.32727911020525	8.87510592945215	11.73295139707751

H	4.36372396266803	7.42633524329461	11.34389056109008
H	4.81598782183635	8.57620886706937	10.05199145303052
C	1.22829356602812	6.33533990213588	15.01044447242685
H	0.53304548533737	5.53827193298698	15.29323183830320
C	1.67851876397696	8.68468330985655	14.56787630657690
H	1.32797821797539	9.71745279903973	14.47351695108638
C	7.04047309930845	7.48065496828847	13.58258537891877
C	0.77479859917196	7.66560761288781	14.92048423968126
H	-0.27455396633501	7.90409861524872	15.11814376763959
C	5.83799431759660	8.48714023366850	15.47840966117819
H	4.95816038308842	8.53001140285972	16.12646184849337
C	8.14574236057325	8.29521307949202	13.88200983574641
H	9.04754136684255	8.23699384541827	13.26364276300804
C	7.57816313534696	8.29388236748600	10.23593707696539
H	7.21081115054153	8.89278587218078	9.38316469983361
H	8.49181123144362	7.77546846999555	9.90190876405971
H	7.85034168688375	8.99804136199412	11.04201052975434
C	2.87270132000865	2.57381657109099	12.18188837134967
C	6.95500519132311	9.27535632849102	15.76044400737164
H	6.93033714649922	9.95525836967394	16.61803733372213
C	6.47523436652714	7.32662605969815	10.69888477636180
H	6.28604020694185	6.57789492572832	9.90489561964362
H	4.97159564306210	4.45276901203345	9.56298613752106
H	3.72748588743501	3.17347294108177	9.36510441012891
H	5.25375063614881	2.82685698017107	10.24343323511771
H	2.66403675256977	6.07279209185639	10.60503987834305
H	1.73012532320069	5.47990421323656	12.00592238078159
H	1.63860851601635	4.61303361734573	10.43279627573208
H	3.61615848033284	1.80438581008271	12.45021869834836
H	2.22849572536811	2.17527841698736	11.37864403231506
H	2.24459963869681	2.77519156110067	13.06589925246922
H	7.71557547089467	2.12076951377273	13.45984112202416
H	6.11943879742877	1.34152474152147	13.30051471462194
H	7.04877828311411	1.16798170560233	14.82465437588465
H	6.61453064845039	4.81366207980126	16.50440957580581
H	8.04422386309775	4.33341037500026	15.55284083690917
H	7.30564556041389	3.16852679570026	16.70162882519398
H	4.10278561932681	3.48392947766139	16.22497148305677
H	4.96512575406336	1.92133967803219	16.35674691246407
H	3.83010356478353	2.20738896527955	14.99958641985160

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[PN]Cu(PMe3)2 triplet

Cu	5.29537942643587	4.98140517483723	13.10334677682859
P	5.93648477565664	3.30083597920348	14.50283287843299
P	7.02108136331739	6.24458547215070	12.24335661225927
P	3.57851368490645	4.35772398944411	11.73322769765901
N	4.85655769980644	6.63749268752295	14.16967896480655
C	8.81329509352295	5.69672926619902	12.01113974532126
H	9.39369758557745	6.57922318784342	11.68158233809668
C	6.79818633073876	3.96834851520958	15.99871290212840
C	9.40609965325609	5.20844739634731	13.34010681876366
H	8.84457957541810	4.33868046429543	13.72399167168485
H	9.37234504312702	5.99896857404899	14.10830871839694
H	10.45891202534193	4.89663588282207	13.20384101809669
C	5.85242717351888	7.58133779337312	14.37752883551352
C	2.70035749990406	5.96482144470429	15.07543845236238
H	3.14232649283397	4.99799825884520	15.33527911875083
C	4.61254801288929	2.28955450075683	15.32913518134181
C	3.53882319133810	6.96189900891520	14.50003961254914
C	2.97846751332510	8.23154817485970	14.19804684748956
H	3.61401646441804	8.98479314653820	13.72401862878306
C	4.08650878992285	4.1165503250328	9.96438325538246
C	2.08685835768649	5.44229310550490	11.55300784568281
C	7.06200612206625	1.93794792748424	13.93358094146465
C	7.99472399722186	9.38904239916121	14.77747647345163
H	8.81686929549564	10.10085566905440	14.92487334025795
C	8.89253471773505	4.61539153016666	10.91861632235973
H	9.93505206186332	4.27080503340210	10.78292445827381
H	8.53213488208934	4.98081802343922	9.94129450262118

H	8.27902644211534	3.73674319309581	11.19259916546313
C	5.35328973198722	7.87641388347805	10.66911146737970
H	5.44461263068765	8.70017547375426	11.39909675899141
H	4.53064023883111	7.22497442443982	11.01250450614538
H	5.06846065605939	8.30990576268066	9.69217324584486
C	1.35152154836452	6.24763123015870	15.36422504725498
H	0.72765080693522	5.48352650727181	15.84170958939889
C	1.62265319330367	8.49317750244687	14.45940922270909
H	1.19780142580819	9.46670392329161	14.19277631279094
C	7.04130418966248	7.48787143185275	13.52511899936726
C	0.80938513567150	7.50417475352766	15.05296897159633
H	-0.24347889044589	7.71647598451715	15.26944592832218
C	5.79088218266054	8.54492091223214	15.40698258883687
H	4.91866220034673	8.54906433307589	16.06769023074033
C	8.09438700644051	8.44296974313631	13.75371711862307
H	8.98235483554523	8.43410227621237	13.11226480598621
C	7.79970572749056	8.05764799356994	10.08818782890143
H	7.49644270305864	8.58242657688418	9.16167491767906
H	8.74274551841977	7.52816914015642	9.86959467279365
H	8.00450969799792	8.82688861724165	10.85434864042348
C	2.77159148218745	2.71456469338801	12.05517047384552
C	6.85965959241885	9.45186792889838	15.62430894639646
H	6.80840039554127	10.17956190297942	16.43881731369233
C	6.68150445512490	7.11300202857341	10.55845871635583
H	6.56200929584124	6.28373239900106	9.83070598215621
H	4.48929918068588	5.06283522032150	9.56759463600834
H	3.24426437257631	3.78690194437209	9.32879948276725
H	4.88978303373533	3.36147336633721	9.91923212007310
H	2.39411501346805	6.45990646240846	11.26318418556149
H	1.57665927814010	5.51394063920834	12.52741138191869
H	1.38572226439837	5.04874734518577	10.79521255848460
H	3.54325906516559	1.92566496802179	12.06721076757763
H	2.01938145644212	2.46267906172859	11.28595085511067
H	2.27757495829093	2.73554870774836	13.04078807346371
H	7.97271031103917	2.36204895776251	13.48175642991683
H	6.54136617674286	1.34923805773196	13.15885333705811
H	7.35170482285948	1.26385039207375	14.76000388099667
H	6.10655213014642	4.65853141785624	16.51049796688977
H	7.68115143177570	4.55328811805054	15.69684125424504
H	7.10349138026664	3.16977583900200	16.69837516193995
H	3.91772358138391	2.95614896973142	15.86651826317811
H	5.04308356245896	1.57626652569870	16.05497210769377
H	4.03725894895681	1.72656375226358	14.57636612666230

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[CF3PN]Cu(PPh3)2 reduced

Cu	6.67125747748417	9.44414281953982	6.19550245417636
P	8.17033877482670	11.03919267601309	5.42684943733051
P	5.93178844631200	7.98583562322861	4.49447710152172
P	5.01929315126692	10.28183842134948	7.62610135154248
N	7.14256054487854	8.23836721072332	7.79089280387067
C	7.46203494609817	12.63575877584496	4.78494042566035
F	4.37951861965895	4.22757663115831	10.33227490020262
F	6.22397709188900	4.74648347171593	11.39913131903312
C	8.42110267212766	7.70984887401454	8.02140527956376
F	4.27167005640426	5.29142508649029	12.24567679064658
C	9.04568486385001	7.74320677260241	9.30077880382560
H	8.49072890184299	8.15487166241925	10.15004169126054
C	6.20975989805555	13.07258966164615	5.25580021484810
H	5.65895752098664	12.44428892812870	5.96132294135306
C	5.22798215241413	8.08443130383168	1.70952191318404
H	5.58257282406289	7.05048923067183	1.64654948405729
C	5.01636585640113	6.52060027812238	10.34063839134520
C	4.98294242417151	5.21006801705110	11.08339561947563
C	8.36902575385250	7.03601526046067	3.41728060596823
H	8.70021054603830	8.07283227976583	3.51711029797987
C	4.67767157546105	6.22798575259032	6.26375046863887
H	5.61891045012729	6.31329842625214	6.81443205722186
C	9.22251191313842	10.56733731183803	3.97050613970997
C	7.06739129345392	6.67067899967693	3.82391210645165

C	4.51120484753303	6.94117030229895	5.05623341116055
C	9.18612597151706	7.19025607273280	6.94498897661315
H	8.72499712415356	7.12900325157000	5.95516508381831
C	2.58939199767640	9.51634348024137	6.44486751856152
H	1.51260896320107	9.70452767979045	6.27655558574502
H	2.69848212135209	8.53581236087061	6.93507520487817
H	3.07891942227778	9.44937686642210	5.45795638919715
C	3.64786713122791	5.41666597829030	6.76182259881388
H	3.79014745404133	4.89142251793638	7.71182618094330
C	6.11876053439169	6.82191164074449	9.53979979310071
H	6.97345534655381	6.14130202011625	9.52439214684122
C	3.20368364682759	10.64905517586016	7.27886348060363
H	2.68599049924194	10.69607552180472	8.25577612984319
C	8.16739363714139	13.46016769934802	3.87894864482672
H	9.14569298932581	13.14428668484727	3.50445181496759
C	7.62184173994977	14.67939561033958	3.45086252520472
H	8.18112236820104	15.30478599365605	2.74644160613987
C	4.96818743385517	8.81905339087377	8.72949273712797
C	10.35650727397137	7.28578542372098	9.48174297848052
H	10.80518354192909	7.33322765941766	10.48135248686766
C	4.33176171276711	10.74217970017017	1.85614522033294
H	3.99226024142247	11.78151075301690	1.91880284972803
C	3.88368236923827	8.49955339850703	9.56743782354501
H	3.00334814729318	9.15129480047994	9.58482159090274
C	2.43968560378464	5.30474391650134	6.05339090243404
H	1.63101111976294	4.67667099056500	6.44262351861882
C	5.28703403592941	8.76909530402927	2.94265847798912
C	2.27108903395206	6.00050126391194	4.84572769954826
H	1.33249604551566	5.91229315634925	4.28720590071766
C	4.72605925003392	8.72288491498537	0.56498595080151
H	4.68831256040762	8.18023674724935	-0.38604223038962
C	3.30064156091428	6.81487017062581	4.34563925808832
H	3.15709943941058	7.35636076666729	3.40549935922642
C	4.83847409223608	10.10587845059345	3.00040837034547
H	4.90384961462688	10.65593765975786	3.94678939541918
C	10.16265140043276	10.67443117614802	7.37699963858365
H	10.00047475099455	9.60702944419747	7.19507020760682
C	7.55584059697501	4.36724540921415	3.16359627870198
H	7.23152620496225	3.32481562593742	3.07206679910719
C	9.41424586051951	11.63933869585757	6.66561899535940
C	10.69139446147968	9.79600068677474	1.67983277044562
H	11.26264795208339	9.50130439267616	0.79301117205754
C	5.66335359975095	14.29427415253629	4.83030832478083
H	4.68516531153396	14.61170656065180	5.20761528337704
C	11.31544296388371	9.85446501954491	2.93536389405076
H	12.37849765647252	9.60827565504509	3.03312427812175
C	8.59773850648989	10.49483831197718	2.70366726143966
H	7.53331303872369	10.73395185259061	2.60875566499646
C	9.61692220982953	13.00677667921343	6.95003881716812
H	9.04016585448720	13.76970607947522	6.41972772936113
C	9.32857735759536	10.11948207717338	1.56794178648166
H	8.82818784651218	10.07322022470304	0.59491591054048
C	10.58914354483863	10.24126093237538	4.07458208255221
H	11.09314440635783	10.29768607144657	5.04376716152238
C	6.13659043470023	7.97618586694212	8.69364313396473
C	10.49928800841029	6.73684494024003	7.13206953108113
H	11.05062393907432	6.33481747706475	6.27395877114277
C	9.24796340324387	6.08103034480328	2.88512881671612
H	10.25160252567693	6.39028384177366	2.57515530469363
C	3.01878508663804	12.00693268038357	6.57965775587782
H	3.47591567316708	12.00091117210541	5.57422178039615
H	3.45493939638304	12.84484361842108	7.15167770462279
H	1.94149044574163	12.21834911119285	6.44822235313376
C	3.88152066273643	7.35698195257691	10.37554448220103
H	3.02828699957664	7.11678558917922	11.01414169221952
C	8.84567015424435	4.74230067207242	2.75901941331269
H	9.53492737570654	3.99470083779963	2.35166681077246
C	6.67097362764224	5.32223142664196	3.68924036172423
H	5.6698868084608	5.01321150605500	4.00189923142965
C	6.36722837932099	15.09958946406435	3.92306473988316

H	5.94282536123898	16.05138530006134	3.58580727136776
C	4.27547238485147	10.05139450687728	0.63545069192548
H	3.88701572743107	10.54825369535397	-0.26013551870514
C	11.10127531479250	6.77998665331159	8.40065216063748
H	12.12561692476405	6.42160466238882	8.54703316124290
C	4.48549942078575	12.00445570221639	9.89177933111318
H	4.27376457823212	11.11245304913782	10.50753130157133
H	3.53211815776984	12.37172700631616	9.47516214291157
H	4.87609511333841	12.78935341010113	10.56610859722319
C	5.53079171369017	11.67983896167123	8.81153126725957
H	5.67579863467649	12.56759824989248	8.16487449326970
C	6.88076748495168	11.33323777913544	9.46391361942633
H	7.23053647939515	12.18490089158405	10.07559183400228
H	7.66155434011745	11.10155906501353	8.72290940143430
H	6.77363491699420	10.45731826471315	10.12675607089264
C	11.30787746781894	12.43493691708086	8.60710959543503
H	12.03929973527763	12.74467278103541	9.36144580319075
C	10.55608802913576	13.39823046781064	7.91673433542355
H	10.69932886874258	14.46359151560730	8.12889113172267
C	11.10922675531225	11.07290249835524	8.33329797870479
H	11.67507964718537	10.30641827405375	8.87210741061342

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[CF3PN]Cu(PPh3)2 oxidized

Cu	6.68198803157349	9.38683925485922	6.16669455663527
P	8.21336754416401	11.02207364480377	5.38351301361685
P	5.84609987308678	7.96063799167725	4.47508038500600
P	5.04474663489824	10.26801922405177	7.63463862714601
N	7.15355716695194	8.22611913190598	7.75681461922764
C	7.46299883790084	12.58454269423657	4.72796573974630
F	4.40672761187032	4.16812467732892	10.24108292293331
F	6.29220267311157	4.64095050092235	11.26078593746880
C	8.44193138550554	7.74237152233550	8.00986669605378
F	4.37275182257526	5.19310374034788	12.18034117931226
C	9.02805884674711	7.77870847369498	9.30774300114492
H	8.45646751209959	8.19626454371557	10.14161567330278
C	6.19740758523282	12.99847817279906	5.18519181277506
H	5.64941228377795	12.36635147571991	5.88918376141028
C	5.19009772379682	8.06213647916394	1.70181797306323
H	5.51407558742241	7.01749660134375	1.65499787177767
C	5.07271556866942	6.44035424078869	10.28125752537952
C	5.04375947980043	5.10974429612822	11.00286633646339
C	8.29643113626009	7.01682696326420	3.44259719998597
H	8.60432984930933	8.06565909842728	3.48017665247318
C	4.54918718525171	6.20021370640802	6.22209492003823
H	5.50607144678011	6.20259081840677	6.75268771313159
C	9.30423105131507	10.55946369695381	3.95879097335537
C	7.00411119921436	6.64222341979906	3.87249863070065
C	4.40186850015550	6.96053563109794	5.04058223169772
C	9.21865200146080	7.24826072415734	6.92819175959036
H	8.76762672096685	7.18899446058103	5.93336356371744
C	2.57053558254198	9.55054277152530	6.52016041203532
H	1.49548773450431	9.76735450975509	6.38682376981826
H	2.66484942757867	8.56283505633382	6.99957728988007
H	3.02685639284716	9.47891033730889	5.51841193246751
C	3.48960065995207	5.42034851783901	6.70748425073181
H	3.62230717898379	4.84386436131948	7.62873720451421
C	6.16885230504097	6.76949849592128	9.48342354134627
H	7.02211340840205	6.08998185469166	9.42780812773270
C	3.23232525473496	10.67031275613603	7.33630377728643
H	2.75041579129724	10.73510625380112	8.33026485219631
C	8.16518506919103	13.41706318833811	3.82739876237246
H	9.15319023403653	13.11944851723074	3.46431152257522
C	7.60168997484989	14.62526883713362	3.39177334375375
H	8.15718971353713	15.25942529316490	2.69317839388487
C	4.99516454243527	8.79279073126399	8.72420364949100
C	10.33816984589099	7.33326948619557	9.50519194356604
H	10.77904101799838	7.38305752970914	10.50608580845208
C	4.37207617362313	10.74989851567114	1.80731920379295
H	4.06364592529019	11.79930150268152	1.85146238446374

C	3.92225496044398	8.45017325024596	9.56417495313726
H	3.04033098919648	9.09542413169790	9.61499133554790
C	2.26733956996766	5.39197752983626	6.01489876477653
H	1.43692061313426	4.78602589271558	6.39146613405301
C	5.26042229997604	8.76608654173031	2.92412008351091
C	2.11664020187723	6.13587688859928	4.83381455811374
H	1.16959129774019	6.10751317694298	4.28486362561413
C	4.71272647132888	8.69923944776792	0.54675569410740
H	4.66289802736098	8.14521272818430	-0.39635283205964
C	3.17689459687382	6.91661397541039	4.34488990973370
H	3.04777362996597	7.49241349908068	3.42360345162091
C	4.85149890290605	10.11615305693708	2.96460264805037
H	4.92467608147727	10.68153997060094	3.90087313137957
C	10.21707144379636	10.72313829068907	7.34449381349656
H	10.18002469054561	9.66065367699353	7.08395804923671
C	7.52704943525648	4.32521418393692	3.30009522878802
H	7.21896582389061	3.27592235661225	3.24528461001570
C	9.38042505102596	11.64656433982984	6.67672501565741
C	10.83209220452654	9.87360170462243	1.68399072904394
H	11.42684603681029	9.61495042522832	0.80198154490002
C	5.63350739838025	14.20856835044944	4.75039021224719
H	4.64667045712617	14.51182561756601	5.11579166295450
C	11.45136769680647	10.01962639632174	2.93444956245443
H	12.53305177158731	9.87924185011863	3.03173764804940
C	8.68461215391764	10.40497190906822	2.69679689119764
H	7.60377192968262	10.55391921227327	2.59794229359430
C	9.43588164590433	13.00824827728672	7.04339095729951
H	8.79685773391293	13.73938794205439	6.54083275833502
C	9.44568329437771	10.07105168623876	1.56766571399264
H	8.95270225758908	9.96373937856246	0.59608326697831
C	10.69521806545592	10.36611336237671	4.06738600506668
H	11.19757698526035	10.50418719734229	5.02900750194521
C	6.15356377317244	7.94776375925180	8.68094870707250
C	10.51923592729345	6.78310418667747	7.14233930076047
H	11.08972473396609	6.37748125797006	6.30085376706695
C	9.18884113941950	6.05635786414379	2.94356111634547
H	10.18184111396206	6.37010325682968	2.60577740074518
C	3.06135163842325	12.03034846348213	6.63543438977662
H	3.46037068556455	11.99907346595807	5.60673373704534
H	3.55205644878005	12.85923122828067	7.17420587687831
H	1.98636853567128	12.27279356538132	6.56160067359358
C	3.94642617767655	7.28430032059519	10.34150592262453
H	3.10193564009286	7.02836240100872	10.98656469142881
C	8.80849529282306	4.70657307694878	2.87503983903241
H	9.50607832636827	3.95613921485332	2.48915551049498
C	6.62698857690959	5.28372810967914	3.79284070328139
H	5.63040378864956	4.96950944288459	4.11368686942162
C	6.33461658105283	15.02358754350043	3.84919559345668
H	5.89805333642926	15.96715335413737	3.50625645446646
C	4.30201315849235	10.04181854870576	0.59737990907530
H	3.93295545893304	10.53645839673587	-0.30689918692568
C	11.08960335814762	6.82662407015737	8.42847603231486
H	12.11060279715033	6.46774086441306	8.59110043852063
C	4.62423700625354	12.04148170393903	9.87202171114387
H	4.35825368166024	11.18148497219190	10.51200282775919
H	3.69741138892723	12.45727705528013	9.44469176523058
H	5.06079530105582	12.81665362536163	10.52742009601549
C	5.65628559262726	11.63625367694718	8.80554590396556
H	5.85595396592149	12.49529280300392	8.13641032498170
C	6.98130887921359	11.22615146933876	9.47018199508955
H	7.39093367540745	12.08447221847942	10.03079853091831
H	7.74569045794372	10.91030739330145	8.74272768641892
H	6.81865296091680	10.40312181637557	10.18793111121043
C	11.15327128589074	12.51522506496560	8.69896129481767
H	11.84158346539255	12.85339780730057	9.48023787278948
C	10.31535089695473	13.43533553159000	8.05066404052794
H	10.34865206552711	14.49541437611092	8.32315563352065
C	11.10336237579232	11.15877951976047	8.34116265089140
H	11.75023530080170	10.43098862619881	8.84113243788913

#=====END

[CF3PN]Cu(PPh3)2 triplet

Cu	6.68985330831260	9.42194795994133	6.20924580935669
P	8.22990380798539	11.02360675197765	5.40834978782545
P	5.88552389204624	8.02321800312372	4.48612726482760
P	5.03907234972422	10.25240723281895	7.66943919832394
N	7.15724139464796	8.22963818463492	7.78622657534636
C	7.46124538284390	12.56952863601748	4.73361894543260
F	4.46126248837195	4.03511564312103	10.06548653565847
F	6.23293143968999	4.56205630575533	11.24446074500125
C	8.44815935082028	7.77345044630941	8.07721582042172
F	4.21131362340148	5.01000502000881	12.01314773588451
C	8.99506075494558	7.84771117769351	9.38886727189271
H	8.37929823293689	8.25465880397351	10.19563476114295
C	6.26454959748219	13.04949384643501	5.30087131017605
H	5.79498178124211	12.48290868330884	6.11000024724035
C	5.14840956239108	8.16081206051960	1.72206758760987
H	5.46056858066246	7.11386906094836	1.65043462180173
C	5.04085208728720	6.35577695756922	10.24075072218731
C	4.99399936573471	5.02071787708795	10.89001374134254
C	8.37328644501924	7.01466377244326	3.56683845504259
H	8.74813492301827	8.02411039106132	3.75459661167277
C	4.64006707909625	6.20646444932773	6.21473906246973
H	5.59551065706155	6.23657835266995	6.74627152907700
C	9.28168749469536	10.49773822580700	3.98691517598597
C	7.02432485227205	6.70105033276851	3.83874716651658
C	4.46415830230136	6.97589356878370	5.04337209924551
C	9.26778891526425	7.27647175665831	7.02976431874887
H	8.84485449906095	7.18500138739489	6.02580946049906
C	2.60494770048707	9.57312957979408	6.44887883218009
H	1.52898152934541	9.77766377407482	6.29494402792044
H	2.70817201830305	8.57438344959956	6.90207265228449
H	3.08714535773588	9.53947758934001	5.45676627448885
C	3.60427319112215	5.39760844311839	6.70321002673400
H	3.75761513153249	4.82795108188419	7.62550796553330
C	6.15427416685595	6.72128154389395	9.44228444195416
H	7.01682723266271	6.05375981631892	9.37883071665950
C	3.23395454718065	10.66785168920129	7.32070388643775
H	2.71917902988878	10.68527001652663	8.30022422315287
C	8.06411776321004	13.31655463907584	3.69278918640518
H	8.99863068701059	12.96918330384274	3.24355369144715
C	7.46822817472886	14.50128789389364	3.23272797921957
H	7.94486765602587	15.06531710907039	2.42326202715275
C	4.96612835527282	8.76920767602466	8.69204366205336
C	10.31298588504596	7.44593298652474	9.63289964845687
H	10.72261837828573	7.52935414321460	10.64532642788783
C	4.35984938265730	10.85340262715923	1.88965179237747
H	4.06189476936500	11.90473779872707	1.96109862130033
C	3.87462319923476	8.38820273279351	9.53150118835536
H	2.98848530655980	9.02738355811764	9.59434222608347
C	2.37826781206971	5.34249292878784	6.01814912861880
H	1.56496008747821	4.71494321339730	6.39833795467365
C	5.24973418858219	8.84018712194968	2.96033180211152
C	2.19875003893529	6.09382438471593	4.84600344558586
H	1.24656870569117	6.04943797577997	4.30553949201403
C	4.66343510316461	8.82449183051122	0.58635148594312
H	4.59628385531345	8.28670540960370	-0.36603757848971
C	3.23406006670602	6.90862902524581	4.35831464669682
H	3.08285960994730	7.49475223453229	3.44660027978151
C	4.85306736811019	10.19584321575260	3.02522139947376
H	4.95240247274353	10.74483988479740	3.96907606776765
C	10.21111186398017	10.79517108354602	7.39947444124226
H	10.07882944522928	9.71749542069585	7.26174004022607
C	7.44027510825460	4.42512026402339	3.04092753801237
H	7.06741923246210	3.41486708056654	2.83915611810113
C	9.45452835762236	11.70411936686560	6.62477106294233
C	10.75330607602953	9.59932844858326	1.74176214189624
H	11.32545046566218	9.25445736700179	0.87381983684388
C	5.67479588929704	14.23935939548490	4.84801705980222
H	4.74801559269614	14.59676770246999	5.30976454221946

C	11.38549337072407	9.75617438297515	2.99073904880031
H	12.45372866107325	9.53836618822525	3.09839016325289
C	8.64995162866604	10.33630803585955	2.72564241869996
H	7.58424153208763	10.56027052820339	2.61555607978808
C	9.62793875865362	13.08836933344962	6.83753056599258
H	9.04469747929622	13.80731676048907	6.25522251683443
C	9.38746940596943	9.89470771793288	1.61580624187534
H	8.88485029308142	9.77701331090386	0.64975364428377
C	10.65646189636542	10.20618627308640	4.10304551388430
H	11.16310059601554	10.33859331770277	5.06384934640760
C	6.13803798883773	7.90653365850317	8.67388438373473
C	10.57663460767380	6.84998398530391	7.29116605244476
H	11.18038850058273	6.44255286362867	6.47331145521866
C	9.24276925245768	6.04725235365415	3.03974236833900
H	10.28348335356821	6.31852830346147	2.83467868738028
C	3.07244911406275	12.05323593357095	6.67194413930630
H	3.54737971022668	12.08516834734773	5.67569619230629
H	3.50349870113206	12.86463965969476	7.28419998498228
H	1.99894897915184	12.27724363289746	6.53107515770168
C	3.90320769074025	7.21284211083724	10.27521996211455
H	3.04816204960121	6.94265160779961	10.90256786098141
C	8.77967794779256	4.74787922733394	2.77689456165982
H	9.45900315596003	3.99139224057870	2.36924417834225
C	6.56732842963561	5.39104564752065	3.56660194562653
H	5.52780460693100	5.12203074768794	3.77319182948765
C	6.27337174277663	14.96649242739339	3.80393442587280
H	5.81186484897290	15.89093824498871	3.44047113388935
C	4.26506733688081	10.17032445635122	0.66346681187744
H	3.88988065382069	10.68577824336503	-0.22692632619896
C	11.10984426844261	6.93722909562475	8.58824880494980
H	12.13594583533568	6.61039663970914	8.78681541612071
C	4.53380726824926	11.91384891500549	9.98148259941548
H	4.34785013378651	10.99492206598302	10.56550452212086
H	3.56703160871164	12.27894698607220	9.59555808930812
H	4.92166563569145	12.68035567932189	10.67847066571260
C	5.56300856825202	11.64877311365200	8.86967825822319
H	5.66985579412881	12.55570999870125	8.24218109518642
C	6.93459552086006	11.31599082444003	9.47700930377695
H	7.28787279119804	12.16072999676908	10.09609998049208
H	7.70047186756589	11.11877719160503	8.70942253610442
H	6.86337638964586	10.42593709025037	10.12675625291614
H	11.30585719995755	12.64154924828883	8.54652495330643
H	12.02052952758291	13.00623252069969	9.29225163597128
C	10.54665697326055	13.55094691321573	7.79206468055479
H	10.67103110779763	14.62894874132998	7.94320316027370
C	11.13665924002145	11.26327136555945	8.34513941260406
H	11.71350700597280	10.54137437835900	8.93260532379893

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Heteroleptic phen-PPh3 reduced

Cu	0.30925379388081	3.98425878823080	4.57758143765358
P	2.29920577853475	2.95765337498391	4.33204726960163
P	-0.80530626609077	4.84546187582203	2.82549432240514
N	0.27760625507840	5.28742822615496	6.19559588379859
C	0.87194423158552	6.47921900228574	6.35683744449100
C	0.78404450601581	7.23480224256818	7.54524014868634
C	0.04185936303742	6.73915297550622	8.61242005908958
C	-1.44143086479713	4.91394776754026	9.50593285177921
C	-2.09927288507495	3.72465904029895	9.30504139044141
C	-2.67689351549966	1.80732184211030	7.78088778574580
C	-2.53003630344638	1.21100008747934	6.53210787071717
C	-1.69064066877118	1.81548428592678	5.57232218250636
N	-1.01084413763430	2.95081031045271	5.80160376667825
C	-1.16800752558237	3.55639760536295	7.02063745164167
C	-1.99248577758203	3.01891403061702	8.05548617599261
C	-0.47643992475817	4.80579338065429	7.23168948347678
C	-0.62467088303767	5.49517178673149	8.47351345504683
C	2.96856258361179	2.1622528769837	5.85955363198981
C	2.07911047558490	1.43822279586444	6.68370353396244
C	2.54544084343452	0.78707763207227	7.83515027351423

C	3.90340841266332	0.86037552059552	8.18421250508361
C	4.79424925385359	1.57713491777265	7.37038597648314
C	4.33393581735656	2.22091807642057	6.21139059368138
C	2.29680833637967	1.59637393529514	3.08723223131718
C	1.85983690925088	1.88790529910439	1.77388580956333
C	1.82985305487341	0.88165988978581	0.79659270269286
C	2.21514066703969	-0.42949970346175	1.12218120168625
C	2.63906939040060	-0.72685394977029	2.42621277796977
C	2.68558512371549	0.27887014264340	3.40507737424353
C	3.66796176504054	4.08484304060968	3.81833035188530
C	3.95326117967728	5.18414601310093	4.66122468063040
C	4.96403302440003	6.09556468180587	4.32547596662818
C	5.69945025768780	5.92560387711331	3.13982151788138
C	5.42544854575314	4.83410818179751	2.30210509822411
C	4.41684253535603	3.91499873104697	2.63750236209299
C	-1.62234095484685	6.43604932373574	3.28128827466868
C	-2.51213866161546	6.44323766833233	4.38037138403666
C	-3.13064463084723	7.63379943419935	4.78586785414825
C	-2.85402093803955	8.83646835220984	4.11371302178515
C	-1.96159030740209	8.83933524232861	3.03162260595328
C	-1.34984402587678	7.64645727070856	2.61255036293597
C	-2.18107568608482	3.75145877292000	2.26071665511478
C	-3.51691166146484	4.18462243875131	2.13572843775218
C	-4.51144822611986	3.29566086126851	1.69546065856134
C	-4.18431997984323	1.97193816428498	1.36573491769735
C	-2.85342780041803	1.53545388051494	1.47620896900353
C	-1.85845583074485	2.41592621484886	1.92532396649706
C	0.09775378255933	5.24315604700486	1.26890667040989
C	-0.49517148089231	5.09413301884605	-0.00344934092975
C	0.21639984662180	5.44814767900721	-1.15981038685503
C	1.51957776417027	5.96162118333443	-1.05971799852154
C	2.11489076854496	6.11670176202885	0.20225620382387
C	1.41077859964885	5.75532969841669	1.36126080741994
H	1.44518455118630	6.84977458966531	5.50102694504080
H	1.29592068150701	8.19873984233625	7.61126458493249
H	-0.04316381724695	7.29951495886903	9.54941049713425
H	-1.53697029007892	5.44615612263148	10.45816685666607
H	-2.72571209181731	3.29709508657628	10.09490180957101
H	-3.31799341274172	1.36007621074761	8.54787829630444
H	-3.05370062059137	0.28428287747049	6.28213179505651
H	-1.56559267675097	1.37330726668626	4.57905637860236
H	1.01966553124704	1.37409997827681	6.41535345172453
H	1.84598644775798	0.22469111299027	8.46258408249744
H	4.26653747981896	0.35797587430080	9.08662211164244
H	5.85559349533411	1.63239594501940	7.63387157103453
H	5.03855876511330	2.77096269459654	5.58105126359602
H	1.55845905631069	2.90910120150252	1.51228102432939
H	1.50260352700514	1.12432809797903	-0.21977846348052
H	2.18692800186760	-1.21554589088040	0.36066907330738
H	2.94348357291764	-1.74627360672055	2.68532068206089
H	3.02658545951764	0.03745815892768	4.41591727245565
H	3.40085835156460	5.30445007048880	5.60037296096099
H	5.18389514999643	6.93572968440239	4.99267360627723
H	6.48895645230462	6.63680189903303	2.87650415895791
H	6.00517057165249	4.68681461800914	1.38484982898262
H	4.21819827688361	3.06369574780736	1.98011513959511
H	-2.73443837141210	5.50794325821891	4.90715095515112
H	-3.83007450109988	7.62321202404780	5.62853297884684
H	-3.33499040090257	9.76680140226629	4.43264373552110
H	-1.74415303517161	9.77259866908004	2.50172223947837
H	-0.66313343456927	7.65827283366879	1.76105647657804
H	-3.78232380024787	5.21749951832122	2.37949455698393
H	-5.54490592324200	3.64560426833100	1.60272733648060
H	-4.96165424192525	1.28342978390039	1.01886043664586
H	-2.58727908155480	0.50705104072277	1.20971200388155
H	-0.82073300307662	2.06719765420649	1.99596328344716
H	-1.51140078513932	4.69733291367173	-0.08873905055962
H	-0.25145928374237	5.32548411390392	-2.14220247748674
H	2.07111202271956	6.23765868656217	-1.96433735269069
H	3.13291465871416	6.50918842162509	0.28927455232443

H 1.89177278860538 5.86431727669601 2.33998476536501

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Heteroleptic phen-PPh3 oxidized

Cu	0.27386042404898	4.00503157802124	4.77661914908086
P	2.27020944021879	2.98289148033313	4.20236921906788
P	-0.61455445958937	5.15099619535349	2.94324709277368
N	-0.34963748621917	5.15078405986492	6.34818325576817
C	-0.12154891495714	6.44967665168987	6.59226011781509
C	-0.57066073171965	7.09727744354617	7.76397628635767
C	-1.31314801057087	6.38038996198939	8.69592499205086
C	-2.34544658724793	4.17891380650768	9.36527364810344
C	-2.55664488284643	2.84676443495363	9.09749276496690
C	-2.15801038218862	0.85321866099904	7.60624587052209
C	-1.55855682892842	0.34286210129331	6.46020237601361
C	-0.80524599145243	1.20355174251616	5.63124122240187
N	-0.65662205198190	2.51098213885548	5.88653423309512
C	-1.24826224529790	3.02493115896433	7.00944010442026
C	-2.00548937833958	2.23030390423265	7.91986071789345
C	-1.05673342959554	4.42831932378676	7.27289017420834
C	-1.58504725190071	5.00505651586846	8.46532437020942
C	3.11686124386934	2.45708739585322	5.74621735341748
C	2.52367121362156	2.65176495701081	7.00969172553290
C	3.20732210049515	2.27715319344321	8.17632966939080
C	4.48395531203341	1.70252442538166	8.08835086010357
C	5.08566897738999	1.51395674029217	6.83181254535045
C	4.41537944195564	1.89885272963876	5.66350132517348
C	1.98952535637577	1.49116555435241	3.18119497416934
C	1.48410198900080	1.65294680628277	1.86831415425888
C	1.25724061127229	0.52968580342131	1.05983649510197
C	1.51212464761101	-0.76069589034679	1.55575941011542
C	1.99614293783516	-0.92667059888367	2.86325063691043
C	2.23599888899058	0.19135424242770	3.67808458730066
C	3.57324799089107	3.97657370895019	3.38367456329893
C	4.03527278685694	5.11651825869015	4.08576840224251
C	5.09266161253028	5.87709663254918	3.57300273213624
C	5.70351049231993	5.50425183751848	2.36115080256740
C	5.25215935139765	4.37044577448694	1.66605747200981
C	4.18661843049455	3.60764802505146	2.16836148429095
C	-1.28234247864031	6.79423467960480	3.40513813937454
C	-2.36595493846185	6.84991184512142	4.31609828961181
C	-2.92127654905412	8.08446410820548	4.67592321096237
C	-2.39079576186815	9.27706419765784	4.15246728119575
C	-1.30818047301790	9.22890209196586	3.25996470578190
C	-0.75421007097303	7.99596626235113	2.88283386692222
C	-2.06397014294854	4.15398152102705	2.42607266765656
C	-3.26895864703805	4.76244244418096	2.00208738140115
C	-4.32842000582019	3.96917125556305	1.53932544963012
C	-4.20136278630351	2.57092120040886	1.49519701623318
C	-3.00519369835949	1.96132655192155	1.90913289903803
C	-1.94203367122234	2.74603747068505	2.37574032358405
C	0.40820121951238	5.39725808509464	1.45106409551293
C	-0.04374240166228	4.97804277335506	0.17836653674731
C	0.72500038495945	5.25667104007811	-0.96086101188602
C	1.93800494103541	5.95587427294255	-0.84399196378900
C	2.39322984056625	6.36900491838874	0.41897135680447
C	1.64055811587947	6.08183768262384	1.56651841716078
H	0.42705050518224	7.00223451448052	5.82358628597866
H	-0.34130941158863	8.15509029054571	7.91492930317022
H	-1.68980161196667	6.86310984300589	9.60373840518880
H	-2.75452606670071	4.63236718262534	10.27360151535257
H	-3.14023834281313	2.22953560961947	9.78774847203812
H	-2.73591075905649	0.20520383725066	8.27334224778300
H	-1.64919682846176	-0.71421615333349	6.19736482281667
H	-0.29329917119693	0.81924053212683	4.74299839551010
H	1.53384379702281	3.10926598539266	7.08169319156173
H	2.74322116933845	2.43793397702659	9.15437483366617
H	5.01646232475430	1.40905604297775	8.99821104248423
H	6.08524712688028	1.07394923225419	6.76151236862485
H	4.90127348849622	1.77004098955461	4.69088395556061

H	1.28607609637301	2.65653979441725	1.47362473477603
H	0.88425233713896	0.66244620234241	0.03948217431936
H	1.33694764351947	-1.63516129439862	0.92155596046456
H	2.20083288152116	-1.93006740243465	3.24957778479958
H	2.63049699124835	0.05421078886738	4.68925790533614
H	3.58958900530877	5.38678298685119	5.05069297866357
H	5.45545780281168	6.74938543005536	4.12562103135041
H	6.54063713305636	6.08996055948477	1.96858251605523
H	5.73886025862017	4.06846036006838	0.73345890347957
H	3.85285313421392	2.71879236889871	1.62586318899220
H	-2.79355961468823	5.92548169147395	4.71937438158816
H	-3.77507570600158	8.11673105043117	5.36003548693925
H	-2.82761131859291	10.24051939978541	4.43284488572106
H	-0.90206399806614	10.15345696472060	2.83821265558659
H	0.06676185865897	7.97179060721988	2.16113460720323
H	-3.37456375373780	5.85050924827215	2.02119759494530
H	-5.25403817596549	4.44774807343843	1.20491579775996
H	-5.03220618742317	1.95735342970317	1.13344906911414
H	-2.89907744535478	0.87280029735123	1.86590614440128
H	-1.00734475835624	2.26243646140057	2.67955407965599
H	-0.99838997702481	4.45410337967164	0.07755272389409
H	0.36623870304998	4.94020769281061	-1.94521357915164
H	2.52763918116524	6.18000845941206	-1.73830370654158
H	3.33886903568031	6.91019084650758	0.51457484682691
H	2.01055545999838	6.39567756405092	2.54816954402276

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Heteroleptic phen-PPh3 triplet

Cu	0.21612535884053	4.00127051377303	4.84408487899502
P	2.16170194539833	2.87326302257417	4.21430667046550
P	-0.59097309763301	5.18436626269302	2.97765541250500
N	-0.36264477262117	5.22840804353414	6.28594938931531
C	-0.15756511989516	6.55841395415859	6.45731385134820
C	-0.55246402436095	7.25146140682751	7.60211545727425
C	-1.23715784855409	6.56500518915833	8.63331331806028
C	-2.15466601303304	4.37240756199705	9.47557974043501
C	-2.33376069263944	3.02155250872731	9.28962460132094
C	-1.93607799926259	0.96105041918190	7.89177440501987
C	-1.35920759549803	0.40936700735471	6.72150915057669
C	-0.67795805885790	1.23757120639048	5.83119717731924
N	-0.56179889028629	2.58100565769660	6.00436939044318
C	-1.13602198816815	3.14038580507833	7.14898424668012
C	-1.82004828831925	2.34289805015004	8.12513261093648
C	-0.99528070476433	4.52949789381369	7.31637896185295
C	-1.47391914045579	5.18576626159314	8.49900536163214
C	0.305737858122062	2.27452806076958	5.70773122701631
C	2.54848953347448	2.50618120309991	7.00096956490380
C	3.27842583620698	2.09668586556055	8.12840890275736
C	4.51424840230716	1.45308685195510	7.97329007749216
C	5.03258833234515	1.22879450478851	6.68590355559273
C	4.31635339106616	1.64576115369825	5.55678641868093
C	1.87445244243207	1.42045362654629	3.13233578985914
C	1.33462730574553	1.64100772920859	1.84292932870668
C	1.06981190036826	0.55720120541390	0.99358703278216
C	1.31806318483557	-0.75610418639326	1.42594153008818
C	1.83385322849343	-0.98231353507245	2.71154686559541
C	2.11342191100644	0.09729379130167	3.56419835572701
C	3.48368536238237	3.86957939603531	3.40793548753560
C	3.96923177776546	4.97924098101121	4.13851160040493
C	5.03090469742837	5.74395874022661	3.63821991922563
C	5.62065812364399	5.40802429033152	2.40686091662787
C	5.14289722752779	4.30635332287268	1.68038533448013
C	4.07698703672210	3.53745590371507	2.17432579800529
C	-1.40799705330436	6.78367513988366	3.37146974975323
C	-2.53384068249071	6.75231087555838	4.22679491057469
C	-3.18830416530696	7.94131567406304	4.57219038509866
C	-2.72599223410260	9.17249430391411	4.07678911726341
C	-1.60921646436444	9.20883857678879	3.22839545253560
C	-0.94982495187785	8.02092906852923	2.87359042069189
C	-1.97322492823547	4.15024743559476	2.34057960360088

C	-3.04104488919586	4.73046407391715	1.61760855643211
C	-4.06666410599185	3.92076269268228	1.10976067430990
C	-4.04220569159330	2.53184647117104	1.32137138632952
C	-2.98783192417879	1.95078029605996	2.04196092694240
C	-1.95808919411238	2.75598067512062	2.55098876282908
C	0.48318615363871	5.52969260611295	1.52965583175112
C	0.13982901630009	5.11949158188435	0.22279324705124
C	0.97060845509870	5.45008495502743	-0.85888913828214
C	2.13973042868967	6.19862622335399	-0.65102309160596
C	2.48903783248210	6.60573669583906	0.64669971058628
C	1.67338017386436	6.26329667161444	1.73461829282515
H	0.32135947128618	7.08270222879301	5.62382231034620
H	-0.35391319868845	8.32359247415207	7.67309460880777
H	-1.58390300840591	7.09619074104164	9.52537730756740
H	-2.53278867790368	4.85770460284355	10.38200627847192
H	-2.86605723371139	2.42877217017271	10.04150763016808
H	-2.45215342405606	0.32364503617549	8.61642187768684
H	-1.41660180567780	-0.66280846865303	6.51726065865846
H	-0.18931753029100	0.82324734447026	4.94268484397446
H	1.58635996622864	3.00772286643020	7.12833390532822
H	2.87549129636078	2.28380212723597	9.12870481981101
H	5.08033618367685	1.13262376832067	8.85378938009911
H	6.00207884202068	0.73582302340410	6.56110126779488
H	4.73791880276550	1.49062384851299	4.55797227566835
H	1.13020406405520	2.66171254181606	1.49907168646488
H	0.66356332878570	0.74011494920217	-0.00631050471854
H	1.10711584391027	-1.60097357886256	0.76274587015343
H	2.02627812576244	-2.00400271725081	3.05449637171437
H	2.52143319533972	-0.08889056446915	4.56199274952926
H	3.53605909052148	5.22483175393572	5.11568807139794
H	5.40913562413945	6.59319614871698	4.21657911091662
H	6.45906865338373	5.99747873187696	2.02184409711397
H	5.60721202439586	4.03366919727077	0.72714837578867
H	3.72184668512622	2.67351753549531	1.60513328128116
H	-2.90012961184467	5.79756660282647	4.61813025912126
H	-4.06177419031460	7.90607666123530	5.23093728843847
H	-3.23896328609963	10.10050872922352	4.34876842305233
H	-1.25113608205748	10.16373230242853	2.83024608487787
H	-0.09145762397710	8.06065166088318	2.19679143645671
H	-3.07122005779526	5.81292059843410	1.45979332578718
H	-4.88966305528435	4.37715243949948	0.55045377100325
H	-4.84914295288648	1.90460937937314	0.92916371692371
H	-2.96846889588280	0.87066033965443	2.21731673708486
H	-1.14462741647929	2.29844073952894	3.12214369522270
H	-0.78084153125577	4.55425767203794	0.05031867600066
H	0.69464094745376	5.13127394025287	-1.86930344269102
H	2.77943805955589	6.46266281117326	-1.49921077124825
H	3.40382677149966	7.18084183140849	0.81745316358885
H	1.96549548616303	6.56679484452290	2.74561423400845

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Heteroleptic dmp-PPh3 reduced

Cu	0.34286082690499	4.00278268346187	4.47346311302847
P	2.36341759010615	3.03518985478217	4.15751888164414
P	-1.05824227158846	4.73486522467364	2.85373794481216
N	0.37096876349009	5.44120171081642	5.99417040589230
C	0.84487112200354	6.70290004703958	5.96111345834007
C	0.75092771021930	7.55674706526653	7.09159519462650
C	0.15842571205559	7.10639489811349	8.26179495918802
C	-1.01052964690600	5.24490852418473	9.47759246270813
C	-1.50784712935469	3.96448922593415	9.47257895253930
C	-1.89420607971278	1.80862253824258	8.24267292068200
C	-1.73864643998380	1.07686543317027	7.07494605419224
C	-1.10867703998860	1.65841016052060	5.94320527198777
N	-0.65339100546186	2.92708725354375	5.96903093451345
C	-0.77751545128715	3.65077932271418	7.12526362187851
C	-1.40366023548807	3.13756349372053	8.30178918409583
C	-0.24008468758734	4.99406840368035	7.13556352951696
C	-0.36762848541602	5.79080485362426	8.31393923489397
C	2.72248203270150	1.80325248803294	5.49310180101296

C	2.47876184904169	2.17728062801498	6.83481275150027
C	2.74466034975242	1.28681254327655	7.88521744888578
C	3.23227344731810	-0.00065206502419	7.61010627382229
C	3.45230819478820	-0.39032726005872	6.28051967339526
C	3.20338686464909	0.50390846138080	5.22709148200680
C	2.68279771535289	2.09509795676867	2.60493107663947
C	3.99330243773196	1.76099141667040	2.19201506735027
C	4.19854959002959	1.00236635313947	1.03054839481476
C	3.10165462740200	0.56207554503535	0.27106677743573
C	1.79792757337849	0.88490871219936	0.67592660375494
C	1.59042881930778	1.64977790424445	1.83451908215370
C	3.79255490267632	4.21394030163741	4.22326372365140
C	4.18428416171205	4.88549295839370	3.04210937408623
C	5.19778767466507	5.85499541157268	3.07587327062617
C	5.83232888642208	6.17277602802117	4.28754302379343
C	5.45187417185439	5.50765529523836	5.46296254243111
C	4.43909983884406	4.53570617941903	5.43411658815011
C	-2.03517863283933	6.19660840335326	3.43664013252784
C	-2.63014555531998	6.13899603991560	4.71809809774705
C	-3.39034731256341	7.21331532274507	5.20281017205689
C	-3.54539418855528	8.37272332543927	4.42647421119124
C	-2.93697999693296	8.44993678342343	3.16474705077145
C	-2.18913291807228	7.37010436294312	2.66878861986776
C	-2.34165763256647	3.50039333283321	2.33907621570496
C	-3.58519643557469	3.40033237925780	2.99587163992610
C	-4.49419490039849	2.38878229554166	2.64705644895025
C	-4.17600439022032	1.46309177375225	1.64174189081878
C	-2.94201528531081	1.55816024958944	0.97843130501378
C	-2.02976787408604	2.56638548263962	1.32426435051950
C	-0.36270265664646	5.29488598106115	1.24166331656761
C	-1.17090184003467	5.43972922436856	0.09042867525842
C	-0.61862552298383	5.91508024390507	-1.10779399892916
C	0.74232224927665	6.25797703894570	-1.17162256575839
C	1.55041571857426	6.12184368144878	-0.03306551279336
C	1.00120261908942	5.63990972886583	1.16546301163816
H	1.15352212072313	8.57133397920500	7.02477039674271
H	0.08699264001152	7.75500278415184	9.14155240124341
H	-1.09539609245506	5.87224588549764	10.37115405543567
H	-1.99394392581877	3.55193436285303	10.36292621464839
H	-2.38478787793546	1.37143144972414	9.11900777633893
H	-2.09925473214145	0.04648091007079	7.01008307626679
H	2.07547752178474	3.17089086892033	7.05894206356859
H	2.56316595994299	1.59758242798323	8.91942228570565
H	3.43460356569935	-0.69873854329983	8.42878868867930
H	3.82547914604045	-1.39532732835844	6.05745620416614
H	3.38435507087233	0.18667915190150	4.19629757692487
H	4.85331622335317	2.10290311669110	2.77687120724054
H	5.21812110068251	0.75286700287479	0.71899896744402
H	3.26473835060335	-0.02989716884067	-0.63531550463308
H	0.93986986779353	0.54468298414908	0.08691667282423
H	0.57062869653876	1.90523118041994	2.14075882077923
H	3.71568103646746	4.62514296395894	2.08740332529132
H	5.49959652818937	6.35566961341775	2.14980616441160
H	6.62561649841117	6.92663531251413	4.31264936570648
H	5.95216674890497	5.73637814859304	6.40982856972127
H	4.16932565853923	4.01353305286035	6.35652454828770
H	-2.49518630326447	5.24882457348936	5.34218758932389
H	-3.85556868507587	7.14650073192668	6.19185083847998
H	-4.13360124214468	9.21435279557556	4.80617868375901
H	-3.04707573742220	9.35373540296966	2.55641619902519
H	-1.72485494374384	7.44405673594267	1.68142089988010
H	-3.85816921488183	4.12488956578020	3.76840923243973
H	-5.46076340916116	2.33322350355532	3.15874048156135
H	-4.88892411998886	0.67853435902464	1.36887836373411
H	-2.69141307487170	0.85138189594411	0.18029385169794
H	-1.08234903193122	2.64862961517467	0.78164076852551
H	-2.23162694617970	5.17178699601839	0.13121045248029
H	-1.25370004357526	6.01968413706163	-1.99355783179513
H	1.17087642666604	6.62868688323766	-2.10835631216034
H	2.61183037551427	6.38703484743698	-0.07803663542617

H	1.63886950219174	5.52819201527075	2.04852846315811
C	-0.91924767499092	0.87324104499337	4.67466049149898
H	0.15622961215785	0.78892180247039	4.43335925191809
H	-1.33011599319110	-0.14420446854547	4.76792348053801
H	-1.41795510529349	1.37149526468670	3.82498985902200
C	1.47067919236426	7.18139257541106	4.68009850537183
H	1.82458559342843	8.22027984498739	4.77053358171980
H	2.32927723932024	6.54634739062748	4.40000630939752
H	0.73558283439824	7.13920703019270	3.85555895192699

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Heteroleptic dmp-PPh3 oxidized

Cu	0.26456369693419	4.07058814408278	4.62465829250922
P	2.30374055677226	3.02680785868253	4.19595534489275
P	-1.00267696827514	4.61676013622916	2.75436367003963
N	0.25062942578201	5.69481402691264	5.96730567754030
C	0.64608734036162	6.97244645889519	5.80764190989017
C	0.68916837321514	7.87669654422373	6.90573364840807
C	0.29057118303021	7.46629270001773	8.16495686010999
C	-0.63224715767890	5.64098338730034	9.61782806016672
C	-1.09676341811617	4.35368912720202	9.74298275595569
C	-1.60048691083309	2.13654505576931	8.68012604382743
C	-1.58962019081911	1.34534634815132	7.54255614566103
C	-1.06692862641896	1.84990244030900	6.32179138010956
N	-0.58765165511888	3.11010974935118	6.23958733546016
C	-0.62041697844230	3.91622583515405	7.35013162242801
C	-1.10896084374693	3.46689540798869	8.61410358849248
C	-0.15641067835819	5.27752680697890	7.21186111691107
C	-0.16552692015104	6.13372923273846	8.35258338156431
C	2.49752187162612	1.51891671433982	5.22232724021605
C	2.31924580195992	1.61539056405376	6.62388011810393
C	2.51191376545669	0.49154011735200	7.43782133698500
C	2.86739665604733	-0.74255047188257	6.86512052384742
C	3.03886652470012	-0.84623038634165	5.47583307314628
C	2.85816740400222	0.27595506951595	4.65328124816459
C	2.68436914831594	2.51766379184730	2.48468661453141
C	3.90722242924232	2.83664911079081	1.85471330795676
C	4.16953488464705	2.36349664729484	0.55994598930348
C	3.22702979791737	1.56642710496547	-0.10912705335583
C	2.01387256347394	1.23558217658400	0.51943430150205
C	1.73930179459250	1.71319993139587	1.80756720865393
C	3.65803849033219	4.15569766739699	4.71470533916293
C	3.81283739988554	5.39138070743520	4.04059500848784
C	4.87310761338699	6.24839153926385	4.36081419076317
C	5.78474406362131	5.89378406237768	5.37045639211183
C	5.63617764248161	4.67298258242030	6.04766595506474
C	4.58271053332726	3.80516053834775	5.72569854501815
C	-1.92114363137807	6.14975772671471	3.19284062981925
C	-2.57880917338019	6.23634159673543	4.44315003331488
C	-3.31705227694905	7.38031564580703	4.77612889457828
C	-3.38857740795865	8.45923122129289	3.87837492272365
C	-2.71736124399336	8.38994443421611	2.64711745732025
C	-1.98351710284255	7.24463729260030	2.30199247357715
C	-2.27192331150705	3.31758958511397	2.46593503646846
C	-3.54506276576248	3.34981582044357	3.07968656126950
C	-4.46794862113051	2.32218066664951	2.83729047297831
C	-4.13390012624507	1.25225771124099	1.99012281850406
C	-2.86975280725159	1.21430500123645	1.37525660142915
C	-1.93984710628114	2.23403992508725	1.61472915922152
C	-0.28461924260488	4.91476811491544	1.09963563952735
C	-1.13097673007777	4.93892065602134	-0.03629255470329
C	-0.60552272512502	5.25165101151530	-1.29705824547251
C	0.76285180677392	5.53821948915118	-1.44169035037160
C	1.60849086165715	5.50679032622732	-0.32225659970594
C	1.08719152949369	5.19684443122604	0.94252813155930
H	1.03030328964940	8.90154757430176	6.73322177646334
H	0.31182917835246	8.15721335750744	9.01428665911379
H	-0.62197243767157	6.31576109446677	10.47961426476115
H	-1.46876334495308	3.98571921047218	10.70436929879678
H	-1.98972051799240	1.74925333853556	9.62771573815195

H	-1.97419259067916	0.32247018347227	7.57111903878556
H	2.05133098481423	2.57388815636612	7.08094034096755
H	2.38958709189695	0.57867031398924	8.52191684082464
H	3.01635031041003	-1.61935360643501	7.50278460868575
H	3.32759156621351	-1.80178734429226	5.02734662636413
H	3.01194576878645	0.18616567271560	3.57479596624497
H	4.65601195227040	3.43980400965083	2.37529492418863
H	5.12234109940384	2.60685178144830	0.07953843250251
H	3.44045319312416	1.19441995425224	-1.11587645310209
H	1.28606987138484	0.60040526086326	0.00465668829834
H	0.79720355884430	1.44470892749150	2.29854774042632
H	3.11538737575154	5.68017475506897	3.24867319470988
H	4.99421424910023	7.19101313478349	3.81764564225658
H	6.61245559105300	6.56399721027656	5.62183806732773
H	6.35284732448480	4.38377663989049	6.82246300352581
H	4.49840636142746	2.84687461533650	6.24364943095821
H	-2.51410122404314	5.41199486754330	5.16174776487313
H	-3.83711912235470	7.43031770359797	5.73789297430431
H	-3.96532054391362	9.35192446410932	4.13921916407306
H	-2.76911030086952	9.22803746150388	1.94510149310320
H	-1.47033256669725	7.20203275797199	1.33770689645278
H	-3.83328867071626	4.19187326073056	3.71408427200930
H	-5.45916882584954	2.36776577573743	3.29895906336644
H	-4.86048634702257	0.45662229713967	1.79889298571377
H	-2.61416829710587	0.39387719233293	0.69733682915760
H	-0.97026342639037	2.21732100922969	1.10812455140114
H	-2.19775597857796	4.71710624623382	0.06738739348020
H	-1.26730395955471	5.27361737277742	-2.16842475877069
H	1.16917175870652	5.78120255673330	-2.42837690395232
H	2.67638289667527	5.71710799526970	-0.43364311231278
H	1.76039599207740	5.14138585292643	1.80228901456801
C	-1.04047129748169	0.99192146686172	5.08854091037456
H	-0.00306205943328	0.84835451353886	4.73631591218654
H	-1.46984967023610	-0.00175353628387	5.28710210308764
H	-1.61731375823161	1.45828556363894	4.27088514816197
C	1.01750440769756	7.46944206955311	4.43840676973380
H	2.00680963112502	7.95791620247112	4.45413228545281
H	1.03309158866082	6.65213956542248	3.70371047699656
H	0.28428655027372	8.22037761745918	4.09354217461928

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Heteroleptic dmp-PPh3 triplet

Cu	0.23341246557561	4.01127561785417	4.77238655251682
P	2.19121713143752	2.79217229941942	4.24565574330428
P	-0.78433827642998	4.96355672678544	2.87525734391366
N	0.09696042049147	5.46696565559621	6.14263679469830
C	0.60460073074738	6.73666863720644	6.16593556730700
C	0.44265229701438	7.57158622421356	7.28057463225739
C	-0.30518833050832	7.14397642001315	8.39719923615090
C	-1.63955443176279	5.31472839432233	9.47839835425319
C	-2.16503008171008	4.04424943686680	9.41856977068605
C	-2.43750384669228	1.88359525143575	8.17021356387988
C	-2.14220973188326	1.12961158572335	7.01266083651656
C	-1.32414649960965	1.65585261539212	6.00667370042032
N	-0.82065509894236	2.93019988823168	6.08429870750489
C	-1.12992245729230	3.70200450637997	7.20934633849545
C	-1.92672694842919	3.18813440456546	8.28758686345109
C	-0.63007835793053	5.01917512887777	7.24968836064439
C	-0.86161067126855	5.85369767903932	8.39598295107404
C	2.87614765544471	1.83215952124564	5.66687113707122
C	2.13729424967437	1.61849219318795	6.84657445132375
C	2.70377146544494	0.90015209828606	7.91315779122512
C	4.00639791500985	0.39305832698983	7.81104885939610
C	4.75277580707183	0.61001451015338	6.63951044353525
C	4.19756702080010	1.33103764411091	5.57527761725290
C	2.17121244133928	1.60921687156163	2.83714332035434
C	1.91389014107188	2.09322250237886	1.53327369117102
C	1.88039084450057	1.21163362509877	0.44199685181645
C	2.07610915450815	-0.16523009685160	0.63985456428467
C	2.31020216562252	-0.65482843638549	1.93363581856113

C	2.36333192495040	0.22359237604780	3.02735929772170
C	3.60692058509241	3.93870606998594	3.92661555434602
C	4.00518441563508	4.75990039947078	5.00909464025017
C	5.09547374920952	5.63089950668623	4.87497635598248
C	5.80081998666399	5.69572964707662	3.66183799343207
C	5.41526173369179	4.87857795056411	2.58756339503877
C	4.32349509865666	4.00388486297518	2.71421031501076
C	-1.71297948994750	6.49769852425746	3.28902145257252
C	-2.46619251860257	6.53845643991077	4.48504619993700
C	-3.21231411223821	7.68042247699144	4.80920282584686
C	-3.20264346696329	8.79633594211438	3.95641413578607
C	-2.44745029470567	8.76577645645531	2.77435781339940
C	-1.70646868133214	7.62270657940954	2.43649877647753
C	-2.07844383230754	3.77160459253253	2.32215694693406
C	-3.45341300674131	3.98556713340432	2.55667747283259
C	-4.39759780176167	3.04443760107700	2.11882860368920
C	-3.98517349190185	1.88439538438264	1.44491323735555
C	-2.61770106857670	1.66272955833390	1.21194278880038
C	-1.66744081325001	2.59286931691285	1.65542455653897
C	0.13610903227246	5.37560816991810	1.33975290636891
C	-0.47716640476070	5.29830085310590	0.06840873537307
C	0.23288737798096	5.67557426576665	-1.08093068541186
C	1.55604756176302	6.13600781063503	-0.97621103659511
C	2.17141892817145	6.21539963807756	0.28289719731076
C	1.46750182685476	5.83572306269028	1.43633335457160
H	0.87734686833242	8.57417586828272	7.25381395112223
H	-0.46193186940602	7.80794247594458	9.25331929075622
H	-1.80995964316623	5.94307260662346	10.35942089052832
H	-2.77667428556578	3.65927130809549	10.24183083847123
H	-3.04740934672658	1.45920122714261	8.97389529135695
H	-2.52447856699647	0.11156964993129	6.90100168481120
H	1.12509769925655	2.01943799872231	6.93720587628356
H	2.12114875198496	0.74382693809239	8.82651363078667
H	4.44579653722647	-0.16474825271951	8.64429350305623
H	5.77351850716803	0.22278285445281	6.55734300080885
H	4.79139307827338	1.51059663165020	4.67300184370818
H	1.74562400605615	3.16305222881903	1.36851717349655
H	1.69776365878538	1.60391989878235	-0.56373928784578
H	2.04648966266922	-0.85252583383397	-0.21155630858344
H	2.46144379855170	-1.72680610855757	2.09647932869481
H	2.56356949278913	-0.17041305216803	4.02774355175934
H	3.48089931738413	4.69127317102150	5.96928108739415
H	5.39991421400923	6.25219077188917	5.72333855406522
H	6.65575086452686	6.37153983831322	3.55914019918654
H	5.97586966257401	4.90681438960421	1.64735892007698
H	4.05214913194805	3.35620478517446	1.87621508306887
H	-2.46919355953506	5.68100645638131	5.16584612267438
H	-3.79535641908466	7.69953902762795	5.73533503332890
H	-3.78057023525623	9.68919465494992	4.21543166136151
H	-2.43457304371798	9.63353906860867	2.10703609129895
H	-1.12417575427177	7.60875618439239	1.51080911555856
H	-3.79093310686264	4.89344001228131	3.06362536405223
H	-5.46194618679574	3.22644796985302	2.29878941466546
H	-4.72623316852247	1.15583829578600	1.10101862659804
H	-2.28644395749444	0.76116523955369	0.68656504137250
H	-0.60464944264141	2.40718468079472	1.46950771913088
H	-1.50802648390706	4.94233646132385	-0.02005239364923
H	-0.25165677019435	5.61364066796009	-2.06075532696859
H	2.10615950064532	6.43110307489638	-1.87550323981052
H	3.20374957454869	6.56772426140439	0.37257144636808
H	1.96297963348314	5.88774715090388	2.41069446411540
C	-0.94381400171475	0.83304263661654	4.80839542556899
H	0.15349159912086	0.72866605442936	4.72892788171737
H	-1.37622940000092	-0.17783792869999	4.86917204097649
H	-1.29403289595570	1.30253253616709	3.87110335853135
C	1.34701634203108	7.22398138717450	4.95174940783374
H	2.22090136937686	6.58284367862921	4.73294567576029
H	0.69426220679327	7.22185561772018	4.06074590109362
H	1.70870344013281	8.25344146550163	5.10037286278310

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{PNP-Cu}2 reduced

Cu	2.18843982269731	15.39083106921874	14.08815452667475
Cu	0.17419017171263	16.58082505752392	15.56581515837144
N	2.12027626132627	15.87606056824844	16.22444883334745
N	0.23749824619679	16.01470648212766	13.51482411266821
P	3.95533305076719	16.72163579513891	13.86483994834058
P	-0.77835469066688	15.22453304755059	17.04684686207611
P	-0.02253693749564	18.71655432387637	14.95869094679731
P	1.66795928663564	13.30032799858458	13.49223670421257
C	3.11356251713905	16.83011349762104	16.55781124669070
C	4.03973731186569	17.34289528880129	15.59666970992139
C	4.99476095911795	18.31009734944525	15.98166360979262
H	5.70089229023103	18.69176662062767	15.23404295432053
C	5.07862263950956	18.78701585795356	17.29445327036595
H	5.83560416557272	19.52787896384170	17.57150851550992
C	4.17451062773212	18.28372669033354	18.24968317942718
H	4.21371252449482	18.63958282473332	19.28587909561722
C	3.21597827129974	17.33639589990650	17.88734579605378
H	2.51859375910644	16.95632717923578	18.63993870482981
C	1.99712873218174	14.85293832246618	17.19643264380841
C	0.72757932970028	14.33522389403487	17.60527259228512
C	0.65679951076612	13.26651458180614	18.52664227009828
H	-0.32610555029860	12.89241568157620	18.83761617617316
C	1.80409932997195	12.70586021482581	19.09749256937880
H	1.72626421907968	11.88684327080757	19.81976240696160
C	3.05721386007694	13.24142977812818	18.74214986934105
H	3.97422617178777	12.83772368459750	19.18688584858603
C	3.14918493000419	14.28202172843658	17.81712018374242
H	4.13229725168201	14.68759586526160	17.56384372089658
C	0.10315246475696	18.46971154856580	13.13860117234239
C	0.13062761333296	17.12861447381253	12.64657249745928
C	0.06477586017041	16.95221662981567	11.23294135201271
H	0.08233106812789	15.93308487463824	10.83506257588288
C	-0.02313812293258	18.03540775668318	10.35757137321296
H	-0.07269278310121	17.85122516797497	9.27805303046394
C	-0.03507420260564	19.35472048611223	10.85013678389260
H	-0.10012331649917	20.20846080929338	10.16803438671070
C	0.03236145403109	19.55151238339207	12.23381920179137
H	0.00442267562815	20.57649894781165	12.62572217575417
C	-0.58666306550426	14.92924371855085	13.12256925267589
C	-0.11255551600414	13.58292088055764	13.11980470691122
C	-0.97071201011217	12.53229958854622	12.72643067646306
H	-0.58843028577903	11.50412914152901	12.71281654270976
C	-2.28831147318382	12.77211400517668	12.31966916485426
H	-2.93320180826126	11.94553162083224	12.00403222902234
C	-2.76376614780640	14.09818981663244	12.31951453231061
H	-3.79336353767468	14.31234318502327	12.01021542469289
C	-1.93622854949609	15.14781041936429	12.72038010260641
H	-2.31718379388811	16.17422419064824	12.71841432969514
C	5.70033884761487	16.11260669751335	13.51262569550180
H	5.90359522670208	16.37509877220396	12.46065643116071
H	6.40350340377480	16.70919681486875	14.12699636523279
C	5.96342490065985	14.60871336387561	13.72018133599412
H	5.17354968260068	14.05738630025303	13.16777414151606
C	5.87309312632955	14.21331633569786	15.20065771690289
H	6.59107969560920	14.79522472559127	15.80881964527577
H	6.09575214732550	13.14087328856614	15.34356776098395
H	4.86162427875843	14.40331274966982	15.59546827173320
C	7.33099279419592	14.22154074005872	13.12516600223048
H	7.39108368977463	14.46582209222326	12.04910102681564
H	7.52081342672638	13.13886708293435	13.23880254069900
H	8.15068060992796	14.75915682310583	13.63795317766115
C	3.97682252365076	18.35188554748706	12.93224028455056
H	3.23070307978995	18.97320259275113	13.45754554439502
H	4.96285311500739	18.83153355032667	13.10177614654588
C	3.64684818263179	18.36987398392752	11.42263066784879
H	2.63826683270205	17.93469620831580	11.29527866662308
C	4.62833300286314	17.57140353411765	10.54780259737371
H	5.66768966792347	17.92956995382073	10.67962417413058

H	4.37311497779145	17.68750053726927	9.47900203459334
H	4.60229250208001	16.49258132388681	10.77387007616470
C	3.59892523988562	19.83565035367648	10.94580434049703
H	4.59216373124841	20.31510304621786	11.04229874471478
H	2.87451167240132	20.42626685298510	11.53215830445739
H	3.29864337455425	19.89480174868602	9.88422444409048
C	-1.91150410066252	13.79056782275299	16.63147227124495
H	-1.33895249100427	13.23528779991386	15.86493726210971
H	-1.98249109269402	13.12753405820729	17.51759474234865
C	-3.92615397691542	12.69690658594996	15.61883617300718
H	-3.28366597481074	12.21467539340530	14.86346431181506
H	-4.92716098114165	12.83855410737462	15.17231507278411
H	-4.03766026527557	12.00253150384090	16.47377515832306
C	-3.33609188478232	14.04511485055315	16.08305057388345
H	-3.24524596643821	14.70218071906289	15.19736539314010
C	-4.29807069127293	14.70141458135240	17.09016155309806
H	-5.32811991356899	14.70503903320398	16.68997930555482
H	-4.03180513848013	15.74738569608018	17.30959887513952
H	-4.31606569844867	14.14526438794534	18.04665213394392
C	-1.50622431813125	15.90734749873029	18.63632907532109
H	-2.43859477055088	16.40599158782682	18.31927823835348
H	-1.80400794595036	15.07024183438598	19.29832479553962
C	-0.63039136202006	16.92800901980055	19.40931266987338
C	-1.52863708163256	17.98317203662742	20.08566319908238
H	-0.92552467900199	18.72083349632975	20.64526524306522
H	-2.22399472322561	17.50677957142088	20.80255564979322
H	-2.13521088767547	18.53318801916974	19.34365581330308
H	0.01290676520720	17.45610043442989	18.67615275705457
C	-1.56842460714897	19.78021914789330	15.05816737875767
C	-3.90727799680935	20.16534386279857	14.16313919074768
H	-4.16327515973079	20.81019064513213	15.02505016542880
H	-4.84192596052375	19.69211048542974	13.81117054322890
H	-3.53097638259841	20.81607894673258	13.35361941622803
H	-1.69332393106249	20.10031467984368	16.10975420487016
H	-1.37233923089559	20.69733227737798	14.46920355680233
C	0.27808597821801	16.25817985672742	20.45656011309561
H	-0.33028593023094	15.74285565366087	21.22436153372802
H	0.89593222194673	17.01324692072458	20.97611274199116
H	0.95087852664569	15.51122657871104	20.00666549136826
C	-2.86520030685791	19.10267949053444	14.56061175433699
H	-2.61409907484409	18.51828592237985	13.65288641758952
C	-3.43942308267420	18.14398278229633	15.61655139106969
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H	-2.68522371117495	17.40074948769299	15.92975055584962
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C	1.30410516351968	20.00007789289466	15.31184279749356
C	1.04314581547090	20.98863422177176	16.47237067166912
H	0.14982820136723	21.59183788981052	16.21446306038576
H	2.23091466999205	19.43157422574805	15.51335146379063
H	1.47104375117172	20.57709206180099	14.38212544955573
C	0.77674654643318	20.27795303681923	17.80883436838260
H	0.60084289487484	21.01008608794168	18.61764719700408
H	1.63965244942429	19.64979616282389	18.09198358182384
H	-0.10713159144418	19.61819979903655	17.75126803975594
C	2.23745370549244	21.95523335286727	16.59832536906882
H	2.05800035552522	22.70383328583830	17.39136010141131
H	2.42021937451944	22.49928113539429	15.65389351513466
H	3.15923241994339	21.40180660738434	16.85485719520891
C	1.56839430845355	11.88080191792358	14.71050545282412
H	0.88206828517616	12.24462875526206	15.49729232654117
H	1.06427341931533	11.02684401238652	14.21248296046380
C	2.86930701736674	11.39013483431076	15.38634496260638
H	3.27403568836640	12.23442040576641	15.97505567344830
C	3.95412160288979	10.92934716499892	14.39824181283224
H	4.81285633063934	10.49459248690416	14.94105862623507
H	4.33821840499112	11.76852436565088	13.79371847385642
C	3.57046444357728	10.15476042621302	13.70740922490294
C	2.52335578403071	10.25080336565122	16.36584137726832
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H	1.77421877926054	10.57435549131201	17.10814939916436

H	3.42211437846305	9.91837086706993	16.91624151650488
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H	3.30407432161251	12.23529569134613	11.99913819883009
H	1.72945519768164	11.42297135392753	11.92664702273001
C	1.91175281841431	13.13259268733466	10.58690030596840
C	2.09050782991909	12.14860972066484	9.41412601044468
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{PNP-Cu}2 oxidized

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N	0.22547003281831	16.02747962021191	13.50745737223416
P	3.94299798152783	16.75255082226055	13.87534481944238
P	-0.72789379741917	15.18036385634249	17.04075695840121
P	0.02544507312225	18.71223515159473	14.96135661716737
P	1.62425439782626	13.30418190471976	13.53035940580459
C	3.14669731120611	16.85518059644760	16.58491890319321
C	4.05339375280359	17.36437487164494	15.61164198404948
C	5.01439208130193	18.32624109293760	15.99121810849875
H	5.72031564952875	18.70603178167820	15.24398471483269
C	5.10266512420470	18.79829280055596	17.30649680438729
H	5.86453746923032	19.53451440243365	17.58020290962436
C	4.20438325705803	18.30270537920367	18.26832139357439
H	4.25238465036741	18.65911901017327	19.30272815455389
C	3.24597876074390	17.35022418707480	17.91336037587462
H	2.55378754519910	16.96844099015059	18.66920863131273
C	2.04705209388088	14.85524635347556	17.23760731775507
C	0.78496082084339	14.33259660221215	17.64488009623619
C	0.72991340275412	13.27733138395706	18.58039488928920
H	-0.24400823527013	12.89699620526488	18.90768726612829
C	1.89169479259558	12.73888499268838	19.14626840208037
H	1.82690622234323	11.93231389970723	19.88280894720621
C	3.13795220805114	13.27358448755765	18.77449253399418
H	4.05977210769028	12.88027271196666	19.21571434728722
C	3.21375516534791	14.31120401216962	17.84216716525733
H	4.19014055842134	14.71973513804566	17.57097359218085
C	0.12874300986729	18.48227560502148	13.13745717752632
C	0.13398925844027	17.15171932939958	12.63111441526919
C	0.06545748235063	16.97033723135281	11.22356306782774
H	0.07313761916562	15.95364014549799	10.82093736296861
C	-0.01103466122087	18.06109849553179	10.35367874904784
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C	-0.01778428178089	19.37425314765363	10.85706345884945
H	-0.08789294326919	20.23108982702633	10.18030382338639
C	0.05601726321941	19.56961078541532	12.24195948094447
H	0.02664594584449	20.59248372953319	12.63651699576300
C	-0.61422180759877	14.94268940495595	13.10305384243421
C	-0.14680280137531	13.59947305635355	13.12028525949011
C	-1.00864971140089	12.55545651218878	12.72139182469414
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C	-2.32006597000668	12.81138225574020	12.30175476955037
H	-2.96771718416340	11.99042483913260	11.97936075714251
C	-2.78708326446392	14.13834298590262	12.29154693428524
H	-3.81079956246773	14.35848883920959	11.97104937502833
C	-1.95078536659047	15.18462221223147	12.68849436676863
H	-2.32169494134349	16.21393293694023	12.67982434762541
C	5.65451523311499	16.07333462501833	13.50945907305710
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H	3.26091951876409	19.01932868156225	13.47725656977515
H	4.98915346472776	18.83426591727062	13.12680743975075
C	3.67420850383833	18.41557899028372	11.43717523194348
H	2.66581953472967	17.98418724725909	11.29431526657574
C	4.66433207497209	17.62854509076214	10.56138305339139
H	5.70320888930070	17.97588705335018	10.71757525022561
H	4.42848122173236	17.77295454237980	9.49239244847976
H	4.62697518534428	16.54417714301808	10.75784147051417
C	3.63552803535599	19.88927319200788	10.98388987362996
H	4.62849122954385	20.36320773388270	11.09765992448343
H	2.90839691242812	20.47631679430046	11.57101774476877
H	3.34933524907830	19.96490994425365	9.92023410108359
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H	-5.26937996336221	14.60051826682099	16.66969583717847
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H	-4.27073030123860	14.07617836061411	18.04714031391588
C	-1.47983408217780	15.96954359791182	18.56105310869851
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H	-2.12630900827864	18.60320640823954	19.20228775228835
H	0.04098027375088	17.52053633881580	18.59912325506784
C	-1.56431453558380	19.69672784433084	15.11166349555211
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H	0.87182497482008	17.12527522753181	20.92724705108111
H	0.95426974525900	15.59929092538061	20.00102587362859
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H	1.48979518521621	20.58136282418610	14.37349771763088
C	0.80351275554521	20.35140529179088	17.80809676478231
H	0.59652726741409	21.09877478622704	18.59385272644862
H	1.69746795183435	19.77676481095029	18.10887539426125
H	-0.04969178758941	19.65033703804668	17.78058301152189
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H 2.33258938581744 22.57815370656902 15.57489616310640
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C 1.49733830142197 11.87523530855150 14.72951273572346
H 0.81105259154490 12.23777743085324 15.51679085922873
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C 2.78174317779160 11.34104316338395 15.40584253964598
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H 3.32282683516356 12.32992597290563 12.05481926291853
H 1.77871657284030 11.46741263532361 11.95057276400510
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H 2.53944490367288 14.96367579922418 9.48702752644353
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N 0.15346069338091 16.03970559534538 13.45787135206044
P 3.84882084092037 16.75358408058971 13.84927061374437
P -0.69507291869355 15.12383923321107 17.01412628823486
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P 1.49686038866041 13.317461463363100 13.48972407653935
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H 5.69057997693198 19.65773568356600 17.50849096403061
C 4.13216156368566 18.31089740497961 18.22512416883343
H 4.20518334834235 18.63608809896673 19.26825383452800
C 3.20911433665697 17.31303106968702 17.87064764279283
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C 2.07228864996760 14.80087059005935 17.12044556241534
C 0.81667426474167 14.25450103511154 17.53742390812101
C 0.80686481489798 13.15232065884281 18.43683060690081
H -0.15100451309924 12.74703521425442 18.78227788945996
C 1.99465687935494 12.61007193110407 18.93525193791334
H 1.96190382317559 11.77486234059212 19.64337535801914
C 3.23204229315008 13.15728984657585 18.53512060183284
H 4.17032140588210 12.74559732591115 18.92152007822687
C 3.26443477885188 14.23505050648722 17.63482037761455
H 4.22310406659148 14.65067365999224 17.31163854413640
C 0.12902803684556 18.49344252472624 13.11119257857557
C 0.09736526397381 17.16301267290163 12.58585502763291
C 0.04614631895630 16.99055378487940 11.18112829542704
H 0.03080245685986 15.97369370268883 10.77822078544324
C 0.01535382850384 18.09026095790539 10.31004979607749
H -0.03111461013463 17.92324426386314 9.22866284609273
C 0.03609266217134 19.40192449390877 10.82833256579435
H -0.00372806955108 20.26507938233769 10.15514882372434
C 0.09476626553380 19.59236202936810 12.21154369927438
H 0.08365434125910 20.61448586725995 12.61008400308871

C	-0.71074698948855	14.97925740446444	13.06469359716302
C	-0.26142978101644	13.62208500506595	13.10307932390181
C	-1.15464437631085	12.58660159278179	12.71946762260556
H	-0.80509669400707	11.54737394648822	12.71742519332328
C	-2.46018151359547	12.86732245364366	12.30702187788174
H	-3.12671868667377	12.05441246195419	11.99915175580407
C	-2.90760223228741	14.20568987181466	12.28179057390968
H	-3.92850036633832	14.44126331335146	11.96287417647053
C	-2.04172266952454	15.24231141577325	12.65907534868575
H	-2.38700848705875	16.28074240769649	12.64173338173771
C	5.49870978908326	15.91067916956182	13.51846187855221
H	5.40480601684858	15.52904076327200	12.48593429544625
H	6.30151611893352	16.67433665689500	13.50486892687439
C	5.88348101807643	14.74201603141524	14.45883425272322
H	4.95090916809721	14.22718185433139	14.77282784343676
C	6.61672092367543	15.22706968719163	15.72244842094669
H	7.57539646261665	15.70948527083613	15.45147081634579
H	6.84960846138520	14.37857264290673	16.39114610706542
H	6.02160714933452	15.96231432718423	16.28709978800238
C	6.75268700720997	13.72080522999111	13.69841794339661
H	6.21756544423918	13.30270199028240	12.82654139246381
H	7.04505384705526	12.87988224632314	14.35294751925116
H	7.68128470670052	14.19421722768924	13.32726023351135
C	3.97949105331758	18.31729507977062	12.82045570010065
H	3.19960583499814	18.96554145684972	13.25874237630125
H	4.95525439635655	18.79492921957287	13.04464529452613
C	3.77777201935819	18.27732905891650	11.28840531905487
H	2.80679267405820	17.78818267072465	11.08207877367918
C	4.88458437791512	17.52542264151273	10.52878350809212
H	5.88411927256607	17.92949305352965	10.77890807067842
H	4.74591207377377	17.63383800539366	9.43800785527702
H	4.88859706785203	16.44646730880776	10.75123471721044
C	3.69423322735283	19.72840798669156	10.77083415907734
H	4.64408504796146	20.26691684526195	10.95333033196114
H	2.88041859557688	20.28483484629971	11.26596304795800
H	3.50141090274594	19.74693485516460	9.68306414700464
C	-1.85628321075070	13.69844993504671	16.65167923781694
H	-1.29975912611487	13.11625536508562	15.89423687287465
H	-1.92350782762717	13.06396809611390	17.55871518996990
C	-3.88080411665456	12.60743156153351	15.65832564308754
H	-3.24415220265939	12.11867660484966	14.90219100112320
H	-4.88279708777513	12.75113745009446	15.21516162607245
H	-3.99070578873670	11.91911259380973	16.51840564734525
C	-3.28312582528875	13.95616104166888	16.11051430886040
H	-3.19781944536425	14.60655578459919	15.21911381950992
C	-4.23606716023980	14.61987444542746	17.12102823802498
H	-5.26510215566372	14.64252962853609	16.71913169899775
H	-3.95407956763834	15.65900581778318	17.35212745217953
H	-4.26443454784039	14.05471578660654	18.07211371335418
C	-1.42776967478319	15.88339556909209	18.57194672166655
H	-2.31796826775011	16.43005929509029	18.21392487147607
H	-1.79402199942461	15.07366336427830	19.23353962579931
C	-0.52582660193179	16.86207568150456	19.36445406286987
C	-1.39649414941031	17.93165861797903	20.05441668873884
H	-0.77403517404435	18.64047637578824	20.62976794158700
H	-2.10975253397549	17.46424138033386	20.75945991232983
H	-1.98252299431030	18.51340528083963	19.32015422754538
H	0.13848822812609	17.38341198201627	18.64502964088682
C	-1.55847804597742	19.71297937132897	15.09057305968187
C	-3.91038054869855	20.10957830459272	14.24318150385645
H	-4.17721198728368	20.67954850273228	15.15313929559575
H	-4.83523224686922	19.64293674207071	13.85814908490835
H	-3.55290817501802	20.82941648417632	13.48539921594879
H	-1.68618700083104	19.97580644015527	16.15765445920380
H	-1.37619476727270	20.66044666371335	14.54686193457775
C	0.35290969629109	16.14535363712625	20.40566951028363
H	-0.27863825948331	15.64652403528424	21.16562820509360
H	0.99897813370304	16.86887361411460	20.93546144734839
H	0.99615624009407	15.37690766036341	19.94895267339074
C	-2.84174928148991	19.04366017335978	14.55336778355962

H	-2.58411098038493	18.53587078022817	13.60252901073559
C	-3.38921841979446	17.99534574379101	15.53534815973921
H	-3.69873935373325	18.47577459788905	16.48357619031610
H	-2.62612836621167	17.23374474379604	15.77443385501400
H	-4.27049438500521	17.47712402870597	15.11757544032814
C	1.30886904708343	20.01538940731274	15.30481666004358
C	1.01533868999272	20.99577996737883	16.46427980615425
H	0.09838714594859	21.56501729876935	16.21291367938543
H	2.24835111953551	19.46890135473329	15.50616627158542
H	1.46781941150858	20.59554263248093	14.37583775983038
C	0.78679540691059	20.27719844574578	17.80358255851719
H	0.56479635539330	21.00156994055254	18.60802089024481
H	1.68413369915005	19.70280041912429	18.09390040039579
H	-0.05715222302312	19.56668516622923	17.74693549514007
C	2.17333483633423	22.00681561646511	16.58116471909036
H	1.97585131192865	22.74318483996749	17.38130677173437
H	2.32286701929703	22.56309915549141	15.63799938805767
H	3.11846036789552	21.48705453595369	16.82221397479073
C	1.41476742374222	11.82938538652760	14.62547175837059
H	0.69625725599947	12.12582150878754	15.41081407404189
H	0.95480416925072	10.99091704046972	14.06298683341791
C	2.71015777921756	11.34047630878587	15.31322223733666
H	3.06966023807231	12.16072178791113	15.96118254510026
C	3.83999185695238	10.96570621655803	14.33969170361454
H	4.69283465733373	10.52747613698934	14.88860562554328
H	4.21999842293157	11.84715310224452	13.79569313823565
H	3.50385171609925	10.21967627354332	13.59486675225120
C	2.36747548782239	10.14072358319715	16.21823967559977
H	2.01210946857768	9.28088713614663	15.61825187547468
H	1.58141013944287	10.40073196962797	16.94775968183385
H	3.25638678046026	9.80996365026212	16.78509507045315
C	2.11078129442806	12.51713239755770	11.89391058659144
H	3.19527753343673	12.33339436080094	11.99852793182010
H	1.62294890182634	11.52368412325788	11.84495110235276
C	1.83890682783066	13.28773748850844	10.58498330795540
C	1.99314818201965	12.34196417860718	9.37760079214425
H	1.79436277630934	12.87539449608312	8.43038740189618
H	1.29348813511277	11.48920746367070	9.43942440938488
H	3.01991241921163	11.93359343140562	9.32188511678422
C	2.76015351508865	14.50830640996487	10.43691053121070
H	2.64797611278957	15.20727341485520	11.28443349411358
H	2.54232437997823	15.06475691173311	9.50805076438050
H	3.81958811713368	14.18936089087827	10.39721462609270
H	0.78790048110607	13.63694160217352	10.61027433439736

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{PPP-Cu}2 reduced

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Cu	1.96326637130849	19.03549706283744	5.56677586890014
P	3.69329613524361	17.45807619735033	5.73469191829493
P	3.59719855067090	20.69378723494071	5.25857764298607
P	6.43385466240292	18.31927690612766	7.22499127116741
P	0.92219980248625	17.69711886063309	4.07972435217287
P	0.98687842659682	20.32701803350554	7.13704114243604
P	6.24465672138544	19.95800188968396	3.54818767721873
C	4.22339825692093	16.55465985261875	7.24676263314216
C	5.34054287906642	17.03366414281886	7.99708783127659
C	5.62815130100069	16.46286252050124	9.25687894652193
H	6.46051976524236	16.85044181414566	9.85487203884874
C	4.87155444095953	15.39641668554929	9.76349029465202
H	5.11360715292134	14.96632835295209	10.74135923931760
C	3.80692100365783	14.88425457140268	9.00083593233267
H	3.21562462590390	14.04174813601394	9.37813835302130
C	3.48320684100183	15.46539529747742	7.77010267354814
H	2.63471348243985	15.08355671766849	7.19229872130364
C	3.23135101121487	16.13140474421062	4.54724289175118
C	2.09573506799726	16.31049053114508	3.69950220169949
C	1.85376650520113	15.38818894383930	2.65717740572647
H	1.00616941286516	15.53979031212041	1.97951201766389
C	2.67545882223057	14.26731320408702	2.47055169258327

H	2.46799493015457	13.56275999923205	1.65792980398663
C	3.76034886295261	14.05681742823032	3.34004228154238
H	4.40280598925478	13.17739304724121	3.21489352213172
C	4.03799378964300	14.98278488761122	4.35133382804720
H	4.90108216216842	14.83095483344873	5.00828701789091
C	3.16995461401028	22.00160947080539	6.47942521138462
C	2.11738551864596	21.77163674605268	7.41727349013150
C	1.91593712500363	22.68648787302122	8.47469049512464
H	1.13442622229171	22.49711784426119	9.21900634588894
C	2.69407451302424	23.84705952397632	8.59246647238097
H	2.51904308988910	24.54498433710632	9.41833161763990
C	3.69316552576098	24.10561303281080	7.63729347161000
H	4.29989072210027	25.01588238969298	7.70873945065803
C	3.93264164013225	23.18919775043462	6.60773661858404
H	4.73094777909834	23.37961116192419	5.88250855576885
C	3.95810415881410	21.61549330312653	3.70819729061201
C	5.03174666919048	21.18754483215141	2.86881673525271
C	5.18802031705635	21.76720431291082	1.59009552718528
H	5.98660053457141	21.41817771586156	0.92594190099093
C	4.34249024249854	22.79462747484570	1.14747349495068
H	4.48317418883871	23.23241985281624	0.15331590602421
C	3.32030879235714	23.25801475434458	1.99467893581573
H	2.66061450367203	24.07007104645512	1.66732895658384
C	3.12636715797909	22.66637457043216	3.24751643924817
H	2.31074862005313	23.00963371104176	3.89295025119605
C	6.94362964653447	19.41480648978782	8.66179567885275
H	7.35790132698849	18.77398256021160	9.46435320312786
C	8.03246653179889	20.40331893089091	8.21046031892149
H	7.65732592702858	21.05321979611472	7.40137540660131
H	8.94044564550885	19.89468835407730	7.84162447053504
H	8.33026803487896	21.05313055640712	9.05400117480122
C	5.70150845551045	20.14643151469643	9.19637788837564
H	5.98058427746278	20.82276975932771	10.02551661116620
H	4.94955281527315	19.43235539476206	9.57055316540152
H	5.22570993787265	20.75174117184714	8.40358168428763
C	7.99140306447454	17.31985958107388	6.79958351967863
H	8.56999191213510	18.01882026142308	6.16313564705740
C	7.57917089947582	16.11025648307693	5.94043100612946
H	8.47235724728343	15.62373957441169	5.50704676720752
H	6.90442192838143	16.40290591856503	5.11719422475981
H	7.04754538356718	15.36367483523846	6.55580835512614
C	8.86418435580117	16.86922534827377	7.98201260259133
H	8.31190956930073	16.17168140243920	8.63548374936145
H	9.22036923382323	17.71214013418251	8.59836966096520
H	9.75585446154971	16.33224519826804	7.60683477412130
C	0.36406064459728	18.30298907065152	2.39276903617011
H	-0.00383821768754	17.43524075450708	1.81130056979866
C	1.56677148452971	18.92148213708550	1.66143989108269
H	1.25770828851665	19.31046678541734	0.67354584538185
H	2.36392069226374	18.17602524572373	1.50579763701989
H	1.99668124245145	19.75805414475489	2.24158810376458
C	-0.78519487546040	19.31358562399844	2.54795222011523
H	-0.45689190044948	20.18981183618602	3.13281977726103
H	-1.66561232440388	18.88017113821584	3.05406452688609
H	-1.11183465213996	19.67434559402372	1.55515137137381
C	-0.57866683658335	16.77179651299047	4.78494369153419
H	-1.20324267213503	17.58861740185759	5.19856696672229
C	-1.41191071752578	15.95051568595891	3.78790255534294
H	-0.81281164839010	15.12943437156813	3.35718466222312
H	-1.81147383712846	16.55912769554382	2.95892316126826
H	-2.27367018659278	15.49114418147044	4.30800968029363
C	-0.10492603335204	15.88559907962761	5.95182341251891
H	-0.97235489696161	15.49379269782260	6.51427155284202
H	0.54505359508583	16.44046013881904	6.65062553011071
H	0.47376293828441	15.02544242624219	5.57242840088645
C	0.60466012100216	19.69996907596264	8.86489228059777
H	0.24058739062545	20.54936893463927	9.47511248764005
C	1.89525843461014	19.14919269150377	9.49329676910671
H	1.68854530726371	18.73905555973375	10.49919688773914
H	2.65818372287605	19.93880344488363	9.59186969236766

H	2.32468766217221	18.34103387084047	8.87370675580030
C	-0.49771641949364	18.62874730138796	8.80555500938246
H	-0.17107916349478	17.76742399691369	8.19806013635562
H	-1.43803843775800	19.01124799174372	8.37122890428192
H	-0.72343357061893	18.25775037530888	9.82236819965303
C	-0.61334271251593	21.17248486026136	6.56188518196710
H	-1.22724453580382	20.32330000705721	6.20077533924664
C	-1.40181579827567	21.95233936883142	7.62629514148957
H	-0.81292715822774	22.80544466848034	8.00585348355046
H	-1.69768578024998	21.32649065734637	8.48540111618190
H	-2.32725444149226	22.36392303326191	7.18094334747946
C	-0.28469802713987	22.07852387275705	5.36093404550712
H	-1.21482336709067	22.42404471182492	4.87332774062412
H	0.33228736244481	21.55540771082214	4.60966566703738
H	0.27904554578035	22.96807142489082	5.69202042590689
C	7.78071650459083	21.03362760083607	3.84809321853982
H	8.44194633514813	20.36598231001770	4.43583295092887
C	8.53256608285148	21.52246885340499	2.59958300221916
H	7.89568722652651	22.18963527167525	1.99297912127220
H	8.87934122009322	20.69602577995259	1.95617453358540
H	9.42378192543052	22.10412554547919	2.90217564711407
C	7.38042294546931	22.22507808136596	4.73783546917364
H	8.28090377834443	22.75549067445375	5.09852143172062
H	6.78823463284692	21.90390471684419	5.61232180644284
H	6.76601287264340	22.94303156159495	4.16708591863834
C	6.68936139442828	18.88619749960970	2.07230086523586
H	7.00436666055189	19.54542318910622	1.24011471034826
C	7.85893343788186	17.95324130873611	2.43002850780836
H	7.58285214288452	17.28437363394446	3.26305292846956
H	8.76698617048745	18.50634505925288	2.72768410382269
H	8.12017961025478	17.32009487041265	1.56205112935815
C	5.44523817000747	18.09334554193002	1.63925519214038
H	5.68829452739881	17.43043939113258	0.78822978440327
H	4.63091909783127	18.76899751983098	1.32981663478099
H	5.06648296873320	17.46647970228212	2.46687779387823

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{PPP-Cu}2 oxidized

Cu	5.15320642561013	19.11186216599002	5.43554277516835
Cu	2.14217670456219	19.03883680673420	5.55968776321387
P	3.69950265421801	17.33192346881276	5.75130412186612
P	3.59387700857338	20.81851012562536	5.24153024213432
P	6.29885162121000	18.36536247571027	7.26761402425259
P	1.05768783494241	17.73917644575891	4.02329423641054
P	1.12822106345886	20.29009282916645	7.18236323170936
P	6.10795734461659	19.90735161840859	3.51713176425804
C	4.21866280127916	16.47512932102981	7.27978413269712
C	5.26852073237161	17.04855584574935	8.05639128620543
C	5.54985652012736	16.52221832526363	9.33430024288446
H	6.33792400152591	16.96803593425241	9.95034528508884
C	4.83978286184925	15.41860425796003	9.83175151485727
H	5.07404431875120	15.02042927441825	10.82408390236370
C	3.84038819056031	14.82150635178372	9.04495546981182
H	3.29428412832001	13.94951238697642	9.42016872915457
C	3.52747241617872	15.34992797801849	7.78637115667010
H	2.73452466866706	14.89603108105127	7.18307406942833
C	3.24018699111072	16.04376425943573	4.53889896514676
C	2.16547551244615	16.30957693396073	3.63978362147221
C	1.92301430618160	15.42219622599323	2.57063590523259
H	1.11559303658863	15.62672532108324	1.85958196349200
C	2.69708997560172	14.26323087664817	2.40589405567716
H	2.49236111383842	13.58336067191990	1.57282065327080
C	3.72287797390915	13.97503354446788	3.32189283873737
H	4.31959757848275	13.06369659389213	3.20888044913563
C	3.99686836031580	14.86055036430856	4.37164672889995
H	4.80978715686547	14.64479604366536	5.07258898867752
C	3.17520660897585	22.08735077092456	6.48856150284774
C	2.19256809662947	21.77320979645595	7.47327300530493
C	1.99604029485273	22.65178319512858	8.55897930806377
H	1.26058993054620	22.41096827346448	9.33388264422993

C	2.72394546630977	23.84741857131291	8.65971126408273
H	2.55579235917182	24.51971566627967	9.50699361820238
C	3.65566273354998	24.18139741843532	7.66235421217388
H	4.21477980662307	25.12093057618683	7.72604390921888
C	3.88482127144117	23.30638038977179	6.59323300550510
H	4.62556692815431	23.55890149404962	5.82759246375607
C	3.94519231340151	21.69520790725472	3.67688104387936
C	4.95461586982275	21.17098072103759	2.81652346884370
C	5.10569136850710	21.70742774616327	1.52088849718366
H	5.86174946972287	21.29889668865997	0.84206845599132
C	4.30531311555285	22.77453574353623	1.08465554289842
H	4.43878727280246	23.18130594442615	0.07724417800618
C	3.34553781694599	23.32466558166040	1.95099553699708
H	2.72944814112764	24.16854079393903	1.62283309873649
C	3.16176415682942	22.78470320314040	3.22999771627180
H	2.39953943402575	23.20125290571667	3.89652450956632
C	6.84336040364098	19.49115775561872	8.65871711903691
H	7.32460608590946	18.86424605720056	9.43345876080090
C	7.87155447999433	20.51065496304551	8.13808142765422
H	7.41909450660074	21.16587479779525	7.37480209275922
H	8.76136691597416	20.03238729460178	7.69369099187607
H	8.21684503424339	21.15215129422844	8.96832648596846
C	5.61296059750543	20.18595662186177	9.26187819370786
H	5.92467966573620	20.89595952956556	10.04880959600015
H	4.92142422366264	19.45644832130039	9.71288731761481
H	5.05991097687098	20.75178089504008	8.48999190232393
C	7.84975573041620	17.39799534857683	6.75951006460750
H	8.37536366252386	18.08778934366367	6.07002194936518
C	7.43942646086995	16.13808162772164	5.97455511516322
H	8.32815856197819	15.68589217042420	5.49970852688539
H	6.69820190520348	16.35650969304739	5.18656579931485
H	6.99721037523150	15.38693651107635	6.65112784968570
C	8.78759354814766	17.02404107238073	7.91978399802168
H	8.27740533852074	16.36463845712548	8.64337625409882
H	9.17708652277537	17.90159175877976	8.46124393869358
H	9.65675034954651	16.46701967043835	7.52517921705376
C	0.46885424624059	18.38498341668392	2.36917819002358
H	0.02629622361935	17.53632805065967	1.81352689831542
C	1.66729471532854	18.93591638903987	1.58135473841834
H	1.32604204706651	19.37168833662704	0.62522841884533
H	2.39749643389589	18.14250721463325	1.35509122407421
H	2.18583188900203	19.72767894826504	2.15237061061975
C	-0.61403235882988	19.45812099917856	2.57705510152755
H	-0.19992430219338	20.33285699798100	3.10599596739168
H	-1.47884899868887	19.08780656717498	3.15410944139184
H	-0.98984478656780	19.80566612529450	1.59825540586514
C	-0.44424327007377	16.87602933217806	4.79699660762960
H	-1.00967004542369	17.70468373493606	5.26720739370289
C	-1.35415783698110	16.13986561602928	3.79915590285406
H	-0.80552501282922	15.33032304434078	3.28700375900685
H	-1.78680735931846	16.80625221595466	3.03513432544340
H	-2.19457655574100	15.67243996219212	4.34378365501420
C	0.02710607740899	15.91408267987298	5.90356084473655
H	-0.83862607050937	15.57303683129141	6.49847231982749
H	0.75441842156464	16.38484446872427	6.58723060405884
H	0.50861836654437	15.02401526670344	5.46377730897713
C	0.71098568214311	19.62179757503632	8.87899072689852
H	0.27219395894654	20.44852467861050	9.46951185822184
C	1.99658193429444	19.13582348239400	9.56565530494385
H	1.75745339901888	18.68678025322429	10.54632979638745
H	2.70159710453451	19.96606393250857	9.73166512086113
H	2.50614264935925	18.36925731133315	8.95373073461402
C	-0.32790145195448	18.49312512802880	8.75929509065826
H	0.08737389428451	17.63973039564923	8.19732828179237
H	-1.25500083501183	18.81582083867195	8.25487216764846
H	-0.60403822041609	18.12952771910069	9.76507683142211
C	-0.47324281203180	21.07591929414890	6.53606371625046
H	-1.03361281670325	20.21907778426284	6.11260621679331
C	-1.33347353455345	21.76810074305202	7.60675254903372
H	-0.78626313196439	22.60599814646324	8.07276845292937

H	-1.66670666547829	21.08267203338192	8.40307257023324
H	-2.23886949778871	22.19060474166834	7.13435928121376
C	-0.14322053576028	22.05718444090956	5.39579906217219
H	-1.07131827161983	22.35495104624084	4.87646356305291
H	0.54574643952866	21.62054926251536	4.65233219706585
H	0.33023521449421	22.97034253660678	5.79513762718312
C	7.64634696547001	20.95034716466758	3.89789399430915
H	8.25854866637766	20.28953399835415	4.54289002192945
C	8.46838985572383	21.36434620286785	2.66560128354811
H	7.87050229603717	21.99622991692497	1.98597614447441
H	8.85395379887827	20.50442068719140	2.09393161315250
H	9.33915995367885	21.96334389654018	2.98865249037903
C	7.24056684474991	22.19256725844388	4.71303626669551
H	8.14191266338457	22.68789005663620	5.11555631550404
H	6.57531172296227	21.94306246202500	5.55761390858180
H	6.71107799032899	22.91943078416571	4.07364020301444
C	6.58900639597407	18.80566980280100	2.08374833517979
H	6.97125759834664	19.45385658765075	1.27225268273373
C	7.70718614992814	17.83936940867560	2.51215733734468
H	7.35375554483753	17.16022815526457	3.30605878527474
H	8.60531332225466	18.36169529668494	2.88431356468058
H	8.01469473939585	17.21783098856235	1.65238990792869
C	5.34765024381646	18.04955455969931	1.58583346827813
H	5.62613154799628	17.35338458780465	0.77445958851148
H	4.58534036023286	18.74295638064360	1.19593534374170
H	4.89046791028286	17.45962016370643	2.40118717732938

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{PPP-Cu}2 triplet

Cu	5.13903014030439	19.11023854667526	5.43360985269784
Cu	2.14982978378896	19.04081936375500	5.55859205381387
P	3.69386583371094	17.32543880028713	5.75761885645509
P	3.59175552638548	20.82581350796922	5.23759593722237
P	6.26254566609871	18.37101291774204	7.28167896624819
P	1.09179911279131	17.74435907017494	4.00479394027600
P	1.16137676030292	20.28941484562711	7.19500807500429
P	6.07171470312097	19.89829410515085	3.50283224812287
C	4.19416860618319	16.47801194092785	7.29066677313830
C	5.24809790301692	17.06595226037523	8.06746421779562
C	5.51395377113492	16.54332954723561	9.36234027047930
H	6.29498751426076	16.99518058661609	9.98424947667980
C	4.80016471941867	15.44639414002984	9.85691528154386
H	5.02867816476643	15.05506931679183	10.85465964126995
C	3.79737715328254	14.83995498279995	9.07098942129030
H	3.24732112717860	13.97222695225638	9.45033848691716
C	3.49159536881354	15.36871603066548	7.80466079651585
H	2.69696768591978	14.92161205428722	7.19781211245840
C	3.25225818833563	16.04029458430919	4.54472587418699
C	2.18115626040677	16.32126345205127	3.63174701857725
C	1.95837439107220	15.42992091386231	2.54734405674569
H	1.16680751216550	15.64124011240015	1.81952193718473
C	2.72929303764047	14.27199700395106	2.39647809309655
H	2.53307686430974	13.59456538509125	1.55778060374697
C	3.74802244845793	13.97225648751182	3.32536391867993
H	4.34272393140413	13.05891935126663	3.21768446601799
C	4.01251168143882	14.86430381718588	4.37938952400476
H	4.81964862811059	14.65498333223868	5.08954708901438
C	3.19010215164654	22.09141888906479	6.48486806801618
C	2.20917151782513	21.76339521817473	7.47973089942979
C	2.02960668374659	22.64661858662298	8.57860806266304
H	1.30698681014096	22.40010335577906	9.36475554396159
C	2.75433062014199	23.84002644826040	8.66928274637777
H	2.59266286821193	24.51041520742466	9.52091271666413
C	3.68172706109848	24.18420120058840	7.66329201586615
H	4.23913733983964	25.12496924636699	7.72422878303599
C	3.90414558473427	23.30281966876437	6.59070438816582
H	4.64082871417870	23.54981397791590	5.81886531496270
C	3.92259415144754	21.69216564325460	3.66977086430254
C	4.93326554661093	21.15118366912460	2.80578811111380
C	5.06317773375757	21.68078450923410	1.49322360019530

H	5.80813203075150	21.26301293010041	0.80657717119479
C	4.25972707380321	22.74165623152810	1.06141723608318
H	4.38378167306411	23.13920195065100	0.04781653178082
C	3.30082833203142	23.30417130117071	1.93038837299402
H	2.68096055502278	24.14434381472083	1.59978096380972
C	3.12871307807594	22.76640540730057	3.21787769852119
H	2.36869517447161	23.17920409961245	3.8899239530307
C	6.82370044425817	19.49739304132342	8.67327348828866
H	7.32441601650971	18.87064052795768	9.43641816649279
C	7.83135489296780	20.53350627033898	8.14652485208221
H	7.35220323770610	21.19980221772706	7.40998933438705
H	8.70903569173923	20.06949513434477	7.66353559891301
H	8.19827931974927	21.16195861330298	8.97883289336692
C	5.59910696247887	20.17612724230911	9.30487660977863
H	5.91887926044652	20.91205936128379	10.06571172745344
H	4.94371544869664	19.43766379067308	9.79308812933845
H	5.00304555459113	20.70927517155880	8.54198619337585
C	7.84110973127439	17.43227629414825	6.77483280278066
H	8.36200741514926	18.12733122339269	6.08545993541666
C	7.44201208988088	16.16797811881741	5.99266472574302
H	8.33267353026118	15.71600584697185	5.51892623104975
H	6.69804499357414	16.38167992565059	5.20571534550806
H	6.99658023978858	15.42045537949007	6.67144637418438
C	8.77797578541344	17.06342386180542	7.93708202708489
H	8.25819036761869	16.41785854118396	8.66692201824376
H	9.16925236857352	17.94560936483394	8.47105430069226
H	9.64635651132562	16.49578822485947	7.55303900582675
C	0.50663893951369	18.39873853118350	2.34782893326961
H	0.04557052166864	17.55875247026255	1.79313812305394
C	1.71264366758385	18.92440701185159	1.55549150955354
H	1.37755641639722	19.37777032219643	0.60422045059365
H	2.41928593893044	18.11231176092632	1.32144183242564
H	2.25766302673733	19.69632579526652	2.12862964575877
C	-0.55119326880746	19.49614408095430	2.55525671186115
H	-0.11362351900872	20.35844484262583	3.08558636078141
H	-1.42194597835789	19.14614075008287	3.13701581130112
H	-0.92182338631970	19.85539064012326	1.57757897246235
C	-0.45028918110143	16.91260575892096	4.75371891216418
H	-1.00965682430448	17.74734560487293	5.22287787655896
C	-1.35386893837249	16.19180979609813	3.73964413051064
H	-0.79519573963291	15.39472236797130	3.21757591557245
H	-1.77834901738096	16.87146359578696	2.98183302085416
H	-2.20012991735200	15.71169371440469	4.26609607551755
C	-0.00649685883331	15.93551859047924	5.85717888435538
H	-0.88173148237144	15.59787614448084	6.44186714504267
H	0.72095075030838	16.39224155633393	6.54997364658979
H	0.47470368176508	15.04706996034147	5.41338076271929
C	0.75296026949479	19.61048046422779	8.89462586922823
H	0.30139871499375	20.42825278077562	9.48885641359806
C	2.04832685000439	19.14844317146491	9.57791688244508
H	1.82172725536563	18.67821861152385	10.55270219237879
H	2.72784544347395	19.99757980888070	9.75225379996417
H	2.58223990470518	18.40726630953947	8.95567255228498
C	-0.26394496612780	18.46241265379185	8.77724564684580
H	0.17138565605641	17.61745067422039	8.21797468886275
H	-1.19355110381748	18.76622749165339	8.26464002103124
H	-0.53866887973606	18.09426180966338	9.78285646609976
C	-0.47661667306290	21.04229370411783	6.57996623659746
H	-1.03115312671349	20.17919183428707	6.15898824765234
C	-1.32909217181388	21.72215713082058	7.66418037501315
H	-0.77528193048622	22.55679357223359	8.12969835414907
H	-1.64581488614700	21.02840202800982	8.46093312979484
H	-2.24433684812455	22.14614037798023	7.20985605656636
C	-0.17191112863484	22.03392369236142	5.44291430376604
H	-1.10624901521001	22.32400924121123	4.92836479046605
H	0.52087105155887	21.60899565205512	4.69619809795349
C	0.29761134840621	22.94786175886609	5.84557256789605
C	7.63843547169321	20.91375854194878	3.88026882239319
H	8.24821152225441	20.24478816207138	4.52091266275896
C	8.45350985117363	21.32975191613702	2.64437950074478

H	7.84278491560944	21.95308409691071	1.96738419375066
H	8.83725553145142	20.46883156471269	2.07170131817526
H	9.32462412493940	21.93607601202471	2.95629190628038
C	7.24525326910529	22.15670291256129	4.69848714692341
H	8.14973667043235	22.65431424562789	5.09385956564714
H	6.58541751212278	21.90544561732484	5.54666335757587
H	6.70451786290321	22.87964482905651	4.06365972769495
C	6.57165823168627	18.79674178470557	2.06949673365255
H	6.96858985151639	19.44440303922430	1.26398451302127
C	7.67598398051084	17.82057800543605	2.51001054892609
H	7.30265801173366	17.14597646036979	3.29849528793104
H	8.57156954385661	18.33545890341864	2.89946739384723
H	7.99242180192852	17.19522674682209	1.65497465686434
C	5.33598786169302	18.04727612516633	1.54940646356246
H	5.6247222226799	17.34442343793458	0.74599617042592
H	4.58807019960022	18.74662406049910	1.14357231944780
H	4.85661992184978	17.46493460333120	2.35726606320354

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(DAC*)Cu(CzCN2) reduced

Cu	0.02625897196143	0.04580747072638	-0.02306975582032
O	3.98852808937750	-2.42380084064112	-2.12339168357529
N	2.10442523603665	-1.38513631212046	-1.29406131571079
N	-0.04476308339421	-2.24328159328356	-1.67374414690136
N	-0.69672183393735	1.38303119726835	1.02984110104124
O	-0.37767515008254	-4.19629638549056	-2.85230115172816
C	-2.03756676276477	1.55916916441884	1.35207905175806
C	0.74896825630412	-1.29007413423182	-1.07940851510431
C	-0.00945887382158	2.41876579262362	1.65243351497677
C	2.97379633520628	-0.39185744058355	-0.66032266861981
N	-7.02378109574359	2.87260844727244	3.00047558287750
C	-2.22650550989235	2.71331787395821	2.18619164113686
C	-0.90368007321042	3.27332398339103	2.38296527455526
N	1.97241616144432	6.67583452189239	4.34596956644978
C	-0.40700044214267	4.37826862524229	3.08432902666058
H	-1.06967514607785	5.04278955318511	3.64710367507056
C	-1.48695139590348	-2.18935029876339	-1.42811223799787
C	3.58664922195017	-0.71238441094524	0.57522694773292
C	-4.60626431618956	2.26878752825870	2.22389595799212
C	2.76616915108730	-2.38737583459365	-2.06783386906443
C	-4.40675622973947	1.12508462268257	1.39571284604946
H	-5.27484167806589	0.52654978549626	1.10512144037398
C	-3.50945894825627	3.06627518771200	2.62089667504616
H	-3.67676732317337	3.94088963736417	3.25689332975402
C	-3.13305802690747	0.76651636345835	0.95859599574242
H	-2.98623496417987	-0.11548198470781	0.32824325136904
C	-5.93049746946354	2.60454959719238	2.65231155071726
C	1.86123158992459	3.77660091676179	2.33103564168018
H	2.93228341875339	3.99820308012937	2.33006481382847
C	0.98274685473783	4.63224966336366	3.05896872990118
C	1.37523534994876	2.67465658846748	1.62996495570307
H	2.05418000058346	2.02484429365576	1.06996210828634
C	-2.31196210592806	-1.55931353352791	-2.39133934243625
C	1.88756493076901	-3.36196917754133	-2.84906341396286
C	3.24884044362591	0.80703966911685	-1.36381536232269
C	0.40907664475841	-3.34081380096845	-2.46797475746047
C	-2.00820123469234	-2.86166674604917	-0.29578446809905
C	2.55425487138571	1.16952624409243	-2.67496096280387
H	2.06612876767176	0.25823261709938	-3.06646146412419
C	3.33153861045076	-2.02200918749338	1.31889238858248
H	2.54196653848665	-2.57603298503440	0.77903138945610
C	4.48376163591686	0.22888753482074	1.11551117768396
H	4.97251731036392	0.01298061630633	2.07104940670887
C	-3.70291742279270	-1.59640153119393	-2.17601205300044
H	-4.36857083083693	-1.11512429923198	-2.89979623535311
C	1.52057750362010	5.75468899287007	3.76659500820783
C	-1.11589899172513	-3.50822034259476	0.76097912763949
H	-0.08808462400253	-3.55947432031281	0.35782349017351
C	-1.76017832865336	-0.87655873693617	-3.64136126238334
H	-0.65715625918035	-0.87327746304795	-3.57097391937229

C	-3.40620870102448	-2.86453707479712	-0.13065263944700
H	-3.84069583368688	-3.36326141564823	0.74142994308601
C	2.43926057442112	-4.79869187731054	-2.67569517394381
H	2.39037754067077	-5.12171020214211	-1.62203291633432
H	1.83892051374717	-5.49478641894462	-3.28020752644027
H	3.49028924949735	-4.82690960339149	-2.99963180549838
C	1.97735110293835	-2.94814666704113	-4.35270979657022
H	1.59236065287090	-1.92799882615359	-4.52463985155698
H	3.03142222640634	-2.98402722607798	-4.67132797040280
H	1.38362115058303	-3.65399318049458	-4.95524196323000
C	4.15181721042589	1.71175234127877	-0.77402883432993
H	4.37485798469325	2.65424943944888	-1.28376821088417
C	-4.24807895788128	-2.24725312356671	-1.06354711110420
H	-5.33349537903608	-2.27117903241343	-0.92094963311004
C	4.77137540873327	1.42471423947952	0.44826073309692
H	5.47912726477981	2.13787678689818	0.88360447939656
C	-1.07170697289611	-2.60774804815583	2.01648467034438
H	-0.36960522948650	-3.00875004452457	2.76829609206525
H	-0.74654655582459	-1.58723698541954	1.74062542090367
H	-2.06809768547696	-2.52333975343642	2.48464059213573
C	4.59937217197913	-2.90701548497148	1.32716517328835
H	4.38834713057812	-3.87579075013697	1.81428966948204
H	4.95704973361080	-3.09766517413733	0.30208506936452
H	5.41730169525539	-2.42103709396525	1.88840917502886
C	-2.21326882539139	0.59662094411673	-3.74045649228314
H	-1.92831221022251	1.16959114793572	-2.84153698138676
H	-1.75065380784900	1.07912092140589	-4.61959666863785
H	-3.30815459556904	0.67830377020384	-3.85747700851075
C	3.53401050922888	1.66240174231397	-3.75935076850148
H	4.33313630592538	0.92471096344685	-3.94530687455194
H	2.99335005594471	1.83463098105968	-4.70666591556614
H	4.01143281775897	2.61751837977732	-3.47885552457457
C	-2.14491522171043	-1.66851942044393	-4.91256656746479
H	-3.23991446712442	-1.67563364131943	-5.05723757179011
H	-1.69146964713734	-1.20613999583064	-5.80753208367666
H	-1.80746815492986	-2.71645804928321	-4.84754786161378
C	2.81461655431656	-1.77250982831372	2.75300137222040
H	3.57013994220952	-1.25858882827684	3.37292134877742
H	1.90193094383298	-1.15240834762073	2.75370786383239
H	2.58132969621730	-2.73281569530644	3.24604871805577
C	-1.54175706654710	-4.95098449927475	1.10144251288670
H	-2.53889360252715	-4.98470343721571	1.57431558677811
H	-1.57153252289434	-5.58244502252567	0.19732940174700
H	-0.82657809349595	-5.39803162510057	1.81419620197934
C	1.43918518223350	2.20389444836311	-2.39841566324430
H	1.85905353404261	3.15174641960320	-2.01851871938200
H	0.86413637721927	2.42310627034574	-3.31524125648492
H	0.74307150698378	1.81818544402953	-1.63031329226267

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(DAC*)Cu(CzCN2) oxidized

Cu	0.01612025186859	0.06724401834186	-0.01259130289384
O	3.98637677034705	-2.45533950464970	-2.06761041445513
N	2.10004981283385	-1.38636425475689	-1.27933721075467
N	-0.04729428105436	-2.23137889164528	-1.67335125561632
N	-0.70725831787103	1.40876311760491	1.04722678188039
O	-0.37004380390682	-4.23401092328011	-2.77126125902824
C	-2.04471528969055	1.56712246375975	1.38365838940866
C	0.75401156938681	-1.29884649769628	-1.08703237964743
C	-0.01555646504436	2.44960164317227	1.65171887847478
C	2.96796636244132	-0.39493784629305	-0.63623596851446
N	-7.00935431093788	2.82258432538636	3.06762269614662
C	-2.23633349186563	2.72219416814659	2.21407258410951
C	-0.90371421126857	3.29989970371125	2.39248815478657
N	1.98117395296862	6.70333036801757	4.29367602381442
C	-0.40416196946799	4.39960065707942	3.07715989620541
H	-1.04799612046642	5.07046079115129	3.65268694556815
C	-1.49183274650818	-2.16685966172540	-1.43306440183159
C	3.57604770675377	-0.72217097868308	0.60113551050992
C	-4.60239465663241	2.22853448432971	2.26068506199658

C	2.76886800752411	-2.41216224745282	-2.04721852014887
C	-4.40113536803781	1.08737226893813	1.43937085154506
H	-5.26191805688928	0.47573694700179	1.15874466491183
C	-3.50915921600524	3.05814412078434	2.65533378518909
H	-3.69605391396292	3.92992686882876	3.28847738880629
C	-3.12131749602476	0.74669826042288	0.99391305009984
H	-2.96104612666160	-0.13650266919826	0.36848997363051
C	-5.92178175872835	2.55488432358411	2.70259029316881
C	1.87019581020644	3.80237949339135	2.28436749539839
H	2.93946724966053	4.02610947916133	2.26411436602340
C	1.00045284540501	4.65049334122984	3.02028320285075
C	1.37030201187840	2.69503350157216	1.59420968590769
H	2.03628895857520	2.04331139562183	1.02097925002814
C	-2.30827133134857	-1.53851951105921	-2.40615501610273
C	1.88750391413694	-3.36588893431744	-2.84860201510414
C	3.24498104664885	0.80613488820127	-1.33791378055872
C	0.41728726585233	-3.36425367430174	-2.44234489880089
C	-2.01907800767254	-2.83068370020567	-0.29694269791506
C	2.57261214716673	1.16224863934984	-2.66298792041455
H	2.10736628186433	0.24533289804853	-3.06877276920006
C	3.34132210483451	-2.04365248522227	1.33113142601136
H	2.56567395433848	-2.61001619818440	0.78306106639593
C	4.46189506335275	0.22490423434245	1.15222171627754
H	4.95368232164840	0.00356789592660	2.10470283034764
C	-3.69989918100069	-1.55497616135765	-2.18645659661577
H	-4.36144575523579	-1.08198311726128	-2.91905438917807
C	1.53765348569918	5.77634106674088	3.71773495283551
C	-1.13548063871048	-3.49716595008646	0.75545642575280
H	-0.11097366948143	-3.57426588309790	0.34811450285225
C	-1.75402489581135	-0.89687305095348	-3.67704541303327
H	-0.65043436181885	-0.89754802984499	-3.61031974452336
C	-3.41760809374531	-2.81417647734137	-0.13103322847791
H	-3.85917789416673	-3.31575469494898	0.73572247990970
C	2.45432219107305	-4.80326718572262	-2.75354783245702
H	2.42958928627896	-5.17611097363824	-1.71615057291945
H	1.85011727062909	-5.47660918072406	-3.37902465289085
C	3.49792560591929	-4.80803599765882	-3.10075207367941
H	1.94227606388015	-2.87831576350095	-4.33628644005093
H	1.54588434269878	-1.85530136210786	-4.45703508164177
H	2.99012462869453	-2.89317862059213	-4.67609276698872
H	1.34538083484888	-3.56389620138576	-4.95858339910711
C	4.13809280405765	1.71402783168891	-0.73643023355571
H	4.37327161326300	2.65213916288876	-1.24856270289695
C	-4.25185575599941	-2.19018941431431	-1.06772241634973
H	-5.33821314374224	-2.21092009481635	-0.93171087804915
C	4.74748371511875	1.42544480745934	0.49166428683300
H	5.45825829341956	2.13427635871220	0.92920332510681
C	-1.06333955989593	-2.59761546240125	2.01038013889619
H	-0.36095680107805	-3.00727490453120	2.75618382927377
H	-0.72331509522165	-1.58059551902424	1.73267119663522
H	-2.05354237172956	-2.49814407542014	2.48901082096795
C	4.62744473326485	-2.90297708029889	1.33982402703261
H	4.42979024561699	-3.88033799924260	1.81369594164416
H	4.99896570219954	-3.07631735926167	0.31700122721265
H	5.43046464214539	-2.40896644679841	1.91445650079983
C	-2.19956909218405	0.57427782450665	-3.82845390698714
H	-1.90673550218309	1.18248195037382	-2.95455832485415
H	-1.73876977502395	1.01990862248040	-4.72699994696245
H	-3.29383597824652	0.65884552172030	-3.94607213341855
C	3.56437415715182	1.67737472471146	-3.72619017682051
H	4.38284485507396	0.95778416465103	-3.89482352941508
H	3.04054822196101	1.83616372481420	-4.68457591842553
H	4.01444619656231	2.64294900000977	-3.43782019110102
C	-2.14777532001881	-1.72873469917697	-4.92077191999508
H	-3.24235440146926	-1.73030714444374	-5.06504836110402
H	-1.69064898962045	-1.30033232308319	-5.82985834476203
H	-1.82139915130341	-2.77750577234827	-4.82340075697066
C	2.81498521362402	-1.81967859898154	2.76643505649278
H	3.55653601009342	-1.29481263049043	3.39348472153243
H	1.88533501634643	-1.22377108443959	2.77432205591781

H	2.60558196547424	-2.78973404168705	3.24965650030947
C	-1.59247438439263	-4.92886229109316	1.10317039550313
H	-2.58399212049805	-4.93975319647909	1.58789907361492
H	-1.64661445797086	-5.55976615461740	0.20052056164248
H	-0.87941395285382	-5.39164868163198	1.80704608473409
C	1.43580057410649	2.17853448345994	-2.40828839219915
H	1.83499908751770	3.13584475150991	-2.02907855433730
H	0.86837403345542	2.38465628424114	-3.33205089002866
H	0.73313036358017	1.78631310240071	-1.64697707120965

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(DAC*)Cu(CzCN2) triplet

Cu	-0.00929653810812	0.16989184380861	-0.12327547157141
O	3.98419587695893	-2.32050998729528	-2.23004233353531
N	2.10182441976653	-1.37054688187555	-1.31658002041790
N	-0.06017310646426	-2.21949342796046	-1.71797499413272
N	-0.70538844828253	1.41854351124125	1.06045732990197
O	-0.42941608229473	-4.09614062552536	-2.98982288326042
C	-2.03873493698392	1.56645605563353	1.41865791101410
C	0.72987169451778	-1.26694613981339	-1.06791317652711
C	-0.00793406553907	2.41854412655113	1.72681035166255
C	2.95161665725204	-0.36382219797448	-0.69956046321908
N	-6.99470625755663	2.76758946663327	3.19301583841532
C	-2.21970039488503	2.67243046851551	2.31630089961627
C	-0.88786417989993	3.22910679987942	2.52048429567659
N	2.01709953114324	6.52339808996974	4.59142560159561
C	-0.37932937286240	4.29144987118633	3.26430574142220
H	-1.02302939646613	4.92784926279583	3.87842522482044
C	-1.49609855111423	-2.12785679754681	-1.50028469505647
C	3.59622011441091	-0.66423510367679	0.52764458901906
C	-4.59212789655200	2.2049795092568	2.34606989238632
C	2.74739169018941	-2.33698699449225	-2.09620296789943
C	-4.40058739941245	1.11105931586248	1.45711067937511
H	-5.26669546238897	0.52196013817656	1.14486475502961
C	-3.49254094976286	2.99348480801486	2.78177542413528
H	-3.66441262441285	3.82960104928492	3.46578780067199
C	-3.12661799760040	0.78180983545431	0.99061542126392
H	-2.97680225105486	-0.07295428051665	0.32440645405932
C	-5.90939661140389	2.51367501233053	2.81170425393421
C	1.88033766413151	3.73512240713627	2.42477223384712
H	2.95087426718383	3.95525254458885	2.41064819525538
C	1.01806252544072	4.54545400796484	3.21444943013704
C	1.37685019512711	2.66699908471960	1.68010893870703
H	2.04173843732378	2.04127672742968	1.07740173021594
C	-2.29666481959225	-1.47612387620861	-2.47281366709708
C	1.88760823666221	-3.41628279191761	-2.76259909001509
C	3.15967576150913	0.86133044228992	-1.38251693347583
C	0.38240349799642	-3.28359288656505	-2.50985604352473
C	-2.05436311789154	-2.75444522677876	-0.35668598713734
C	2.44803646423458	1.19215985744291	-2.69200799670554
H	1.94775962624078	0.27241651677552	-3.04210532153014
C	3.41269458253894	-2.00132785860622	1.24024431985270
H	2.60005878100310	-2.54456400958971	0.72626102942646
C	4.46335795405947	0.30639864903337	1.06556727397164
H	4.98338405646728	0.09670553018066	2.00625161910271
C	-3.68937443925065	-1.45468417852453	-2.26505867087850
H	-4.33371588500327	-0.96852510750690	-3.00513533544103
C	1.56536142965653	5.62951926567722	3.97122903320482
C	-1.18666975729016	-3.43087469193658	0.70067838132381
H	-0.16200518351351	-3.50116897457008	0.29627633739701
C	-1.70581452616045	-0.86368131223866	-3.74039971453271
H	-0.60676569800758	-0.85951676035045	-3.62879606883651
C	-3.45277245732567	-2.70224356293221	-0.19701304879889
H	-3.91068551749295	-3.17766748162943	0.67682433239679
C	2.35146176507467	-4.80474908608284	-2.23776102422432
H	2.20017017417865	-4.89373896226778	-1.14752529532641
H	1.76861125201556	-5.59624438709439	-2.73481638348159
H	3.42375121078267	-4.93690070725467	-2.45190774063399
C	2.13257848845698	-3.35648464553998	-4.29681402012892
H	1.81288771509155	-2.38694535979809	-4.71775080907349

H	3.20757506715650	-3.48537939547091	-4.49954800882517
H	1.55812096705547	-4.15619070878625	-4.79048388293530
C	4.03301563159638	1.79917713410094	-0.79836211752196
H	4.21329539622099	2.75307256057096	-1.30535317884994
C	-4.26567482309656	-2.06569129708637	-1.14405836790508
H	-5.35312398629319	-2.05107870259414	-1.01133371754645
C	4.68788521237549	1.52308381070878	0.40921926413388
H	5.37904527272004	2.25723239245579	0.83776885461792
C	-1.11879078531815	-2.54417408250930	1.96437008220067
H	-0.42966324668849	-2.97239060727650	2.71356284989102
H	-0.75442622178153	-1.53621825425099	1.69242605413787
H	-2.11253372316383	-2.43386644654703	2.43486948740515
C	4.69717332984570	-2.85499850994670	1.12606897512392
H	4.54115342601731	-3.84794914865110	1.58497685806211
H	4.97996838885596	-2.99224834164902	0.06979978142811
H	5.54162743998152	-2.37098622055417	1.64968734863764
C	-2.15616898738501	0.59743301718626	-3.95163389053739
H	-1.90466426462223	1.23060690981290	-3.08251295224666
H	-1.65914228348350	1.02323484137104	-4.84133389586290
H	-3.24553833366882	0.67183734177445	-4.11894266234683
C	3.42413114283829	1.63884950492347	-3.79988525157979
H	4.19992078296322	0.87417211519943	-3.97259306376018
H	2.87785416663361	1.79897163924646	-4.74634511808524
H	3.92990882367844	2.58769215147793	-3.54698238763825
C	-2.04876349625704	-1.73829908459891	-4.96929168487058
H	-3.13916875227089	-1.75567471394660	-5.14866911878073
H	-1.56401983788263	-1.33492472887520	-5.87664580602859
H	-1.70883573582985	-2.77529636226884	-4.81585723431568
C	2.98683504969520	-1.82240961365829	2.71328645255624
H	3.76938138251805	-1.31922353779732	3.30902273240031
H	2.06137467760994	-1.22647616247008	2.79750182516689
H	2.80432897185468	-2.80768926098631	3.17781041721817
C	-1.65717082055415	-4.86314253277217	1.02660496378764
H	-2.65992463335219	-4.87394178483397	1.48992050755473
H	-1.69514187301687	-5.48358758044904	0.11543383276741
H	-0.96068370850894	-5.33764246978447	1.74045857418886
C	1.34766694726736	2.24604285163171	-2.43897856815755
H	1.77144169033812	3.20243667694000	-2.08339073141947
H	0.76320395864306	2.44462870043386	-3.35439448390329
H	0.65170692246753	1.87748408219649	-1.65797047753787

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97

(DAC*)Cu(CzCN) reduced

Cu	0.02750886413730	0.04572970320574	-0.01609874003497
O	3.98805227799916	-2.41360974262918	-2.13525428408679
N	2.10514250144405	-1.38377213794118	-1.29272598521026
N	-0.04518518965949	-2.24062849146255	-1.67256917774351
N	-0.69724176055945	1.37548764561131	1.03477482505922
O	-0.38177338005564	-4.18169855685814	-2.86952900823725
C	-2.03710843302167	1.55173813745583	1.34825031725764
C	0.74807806430295	-1.28631597487716	-1.07422027038456
C	-0.00978129423052	2.41569757355942	1.67006142075580
C	2.97542282298953	-0.39302490534256	-0.65786808955697
N	-7.03066355765920	2.87232529823713	2.97453127034672
C	-2.22913948357637	2.70498931911530	2.18624625328889
C	-0.90805278671917	3.26447593655681	2.39471338793723
C	-0.40990635519873	4.37106743030979	3.10546100819695
H	-1.08772653745236	5.02735604080873	3.66286596143323
C	-1.48677909726376	-2.18841539648999	-1.42606622545200
C	3.59173391547705	-0.71803574500840	0.57459669401908
C	-4.61204796443244	2.26203313284133	2.20716299726503
C	2.76475305021150	-2.37953646603253	-2.07184134980114
C	-4.40954542006350	1.12070086415060	1.37632933771018
H	-5.27646011071245	0.52397409846981	1.07824687237029
C	-3.51468796539029	3.05626257903346	2.61296866582675
H	-3.68496688439552	3.92905585590350	3.25102190161203
C	-3.13311772286021	0.76276562401039	0.94634989773706
H	-2.98389794959576	-0.11738133099606	0.31381198315866
C	-5.93685071811910	2.60012462036407	2.62975731686990
C	1.84722956667693	3.77859842371019	2.37348248656521

H	2.92169911828114	3.99285791421361	2.37540976929731
C	0.96829897873712	4.62269444071154	3.09084831952042
C	1.37265714437365	2.67175023490388	1.6589906894078
H	2.05558134576898	2.02315556759175	1.10147179412059
C	-2.31336617868398	-1.55783906889885	-2.38741153689829
C	1.88600310469036	-3.35632798756801	-2.85050028185596
C	3.24788088142906	0.80919827831898	-1.35614471197109
C	0.40611807575286	-3.33075235856035	-2.47395004028157
C	-2.00712377954755	-2.86263597712068	-0.29460469039768
C	2.54822786093533	1.17822175764298	-2.66262688567894
H	2.05228280151099	0.27059287054562	-3.05260720386448
C	3.33553707195458	-2.02954839166207	1.31435065503628
H	2.54254862527703	-2.57875976670068	0.77481312845789
C	4.49160824389755	0.21986400917048	1.11565915068367
H	4.98264031787441	-0.00025456268659	2.06914157090608
C	-3.70426841025063	-1.59861149234647	-2.17293526066316
H	-4.37068159387135	-1.11657665835091	-2.89558916487073
C	-1.11344284754128	-3.50754243944203	0.76193065597899
H	-0.08497527008492	-3.55263146437675	0.35982494597939
C	-1.76212257174908	-0.86846039887084	-3.63394035839761
H	-0.65912497356445	-0.86684413432667	-3.56415564983525
C	-3.40510874567884	-2.86908829111911	-0.12969747765161
H	-3.83848935348320	-3.36878653613586	0.74242760442649
C	2.43344304168758	-4.79329529444021	-2.66326570387495
H	2.37970345723292	-5.10755567743223	-1.60708820852289
H	1.83324335379515	-5.49265542584082	-3.26427673002031
H	3.48573677499207	-4.82667637903608	-2.98283761711443
C	1.98317910865386	-2.95608096908285	-4.35661607834031
H	1.60128559263545	-1.93634164805659	-4.53792656603392
H	3.03841323259656	-2.99663760284848	-4.67082999350355
H	1.38969723359429	-3.66496325840007	-4.95582552914866
C	4.15329507491173	1.71093088318542	-0.76584305283387
H	4.37325247583789	2.65631224601295	-1.27169248076215
C	-4.24832297519393	-2.25284249191477	-1.06194243693821
H	-5.33367472548659	-2.27872417381047	-0.91908202087945
C	4.77747778712709	1.41823824011229	0.45248636472824
H	5.48625107252714	2.12980423069786	0.88890074933354
C	-1.07514398073268	-2.61009982676118	2.01979515110551
H	-0.37308669087881	-3.01101506323037	2.77187410945164
H	-0.75293092596909	-1.58797279465090	1.74703301709971
H	-2.07278024035478	-2.53039956833475	2.48615013728872
C	4.60052175831685	-2.91850290978555	1.31482873358604
H	4.38869131215527	-3.88848683577953	1.79941448501677
H	4.95328532527207	-3.10641635057335	0.28750822391102
H	5.42224478322815	-2.43680612934206	1.87445007273726
C	-2.21381245485217	0.60582305730964	-3.72243150838812
H	-1.92699390641342	1.17170987875602	-2.81967727060066
H	-1.75184432474897	1.09403182959201	-4.59888392937483
H	-3.30888167144028	0.68927196258320	-3.83702883831492
C	3.52599981080345	1.66589953627178	-3.75118950567233
H	4.31811872234198	0.92213110120426	-3.94321303472684
H	2.98177860638220	1.84508816003155	-4.69526687135169
H	4.01282299564719	2.61633841110720	-3.47049395576218
C	-2.14828023119683	-1.65201271812493	-4.90975820707721
H	-3.24345151246454	-1.65790321643888	-5.05372311989487
H	-1.69532315566677	-1.18425946788242	-5.80229072932071
H	-1.81073780715374	-2.70028639956211	-4.85104337149249
C	2.82361928190197	-1.78347858943417	2.75077578331290
H	3.58345778665843	-1.27568250372998	3.37067478406699
H	1.91435925631687	-1.15853085126660	2.75587326161572
H	2.58677582968568	-2.74469871118180	3.24053867073152
C	-1.53330835829662	-4.95320881312176	1.09752794346699
H	-2.53156710502282	-4.99268508517495	1.56773477025605
H	-1.55806812118458	-5.58241958303859	0.19161284614466
H	-0.81786643840875	-5.39899889706691	1.81095304377697
C	1.44116302906988	2.21904026223190	-2.37853576125130
H	1.86815638568886	3.16267173384189	-1.99612140206870
H	0.86483265732288	2.44499718291236	-3.29305936747272
H	0.74533234810573	1.83499967054830	-1.60967763322993
H	1.37000640967557	5.48049062530619	3.64046149745798

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97

(DAC*)Cu(CzCN) oxidized

Cu	0.02177949926784	0.06765158371816	-0.00583072104325
O	3.98522048249595	-2.45575987666159	-2.06936453437775
N	2.10082753991725	-1.38640970736902	-1.27704924338671
N	-0.04766348613473	-2.22890971626112	-1.66967873552090
N	-0.70509450385941	1.40861690844031	1.05206109813954
O	-0.37256875783228	-4.22772136764963	-2.77412538263503
C	-2.04376314978835	1.56179596659805	1.38259450151138
C	0.75440183403405	-1.29677197394269	-1.08182391328648
C	-0.01834523227487	2.45426756272744	1.66172559592080
C	2.97106127654985	-0.39831450831876	-0.63235124337004
N	-7.01822425801254	2.80101885009408	3.04836015888483
C	-2.24107089073917	2.71676074294056	2.21339495939557
C	-0.91171586865395	3.29940410091264	2.39788959076727
C	-0.41056192880192	4.40251104050085	3.08501574249455
H	-1.06744948818547	5.06597791033311	3.65607635584279
C	-1.49202693174728	-2.16630856739509	-1.42836599158737
C	3.57840980636303	-0.72913679932221	0.60421881683421
C	-4.60657964218817	2.21392643476047	2.24952778156684
C	2.76747584170194	-2.40997424672640	-2.04760999688797
C	-4.39921663902830	1.07387816539713	1.42830181962352
H	-5.25685728681662	0.45966080840922	1.14377903112668
C	-3.51771443095436	3.04660930017690	2.64876595705166
H	-3.71030315155210	3.91737039849438	3.28160757340062
C	-3.11610101042033	0.73848431571673	0.98812250108808
H	-2.95000968185537	-0.14334966057713	0.36237409069083
C	-5.92886600099696	2.53608168523028	2.68678229667790
C	1.85434968435651	3.82014190770919	2.30863209714428
H	2.92510087560617	4.04147156395624	2.28831723132463
C	0.98325844146271	4.65579671420492	3.03383806475570
C	1.36670799848575	2.70473569428191	1.61032355130630
H	2.03546753011392	2.05376559699169	1.03906831933665
C	-2.30950981643555	-1.53585892942205	-2.39908093379562
C	1.88437156191119	-3.35950932416015	-2.85190171841726
C	3.25138205527584	0.80302221352817	-1.33191206905419
C	0.41495294981795	-3.35867653295377	-2.44271258069477
C	-2.01855030653339	-2.83611791285354	-0.29551737928350
C	2.57831016486568	1.16389268749576	-2.65528321004577
H	2.11012583279339	0.24908309776869	-3.06243373476908
C	3.33864860332661	-2.05057157123616	1.33266932446253
H	2.55977702651865	-2.61252363827431	0.78470055515853
C	4.46752323564735	0.21398697736363	1.15638021420187
H	4.95817146106637	-0.01017574846429	2.10880686662641
C	-3.70127131623612	-1.55776224721879	-2.18119793056148
H	-4.36339448133285	-1.08265667695530	-2.91193630171052
C	-1.13347145265212	-3.50172858382163	0.75611108706910
H	-0.10927925543665	-3.57773437350487	0.34769372062917
C	-1.75564882478954	-0.88476327542676	-3.66532343185752
H	-0.65214235626421	-0.88381483602211	-3.59767707227410
C	-3.41719265345617	-2.82484210063762	-0.13109960734236
H	-3.85800036667789	-3.33022879771658	0.73380229102485
C	2.45038378392851	-4.79750788149986	-2.76461474990847
H	2.42732857779032	-5.17495486815427	-1.72882876934439
H	1.84445750407224	-5.46767714080457	-3.39183753027076
H	3.49339515121073	-4.80134262168251	-3.11363148155458
C	1.93652963203763	-2.86500511395651	-4.33719105763431
H	1.54012535443807	-1.84131845049618	-4.45203137928133
H	2.98370951688787	-2.87836535781998	-4.67918474523923
H	1.33813574435237	-3.54728139058724	-4.96170666497236
C	4.14738129793511	1.70706334225490	-0.72942303187595
H	4.38371153467672	2.64605472895915	-1.23940527390148
C	-4.25245663141378	-2.19986618391066	-1.06611577360681
H	-5.33883047020836	-2.22391013968613	-0.93086456532926
C	4.75624715281528	1.41468161988216	0.49781317788903
H	5.46791077079418	2.12149393143475	0.93710626211164
C	-1.06125343111188	-2.60141197588069	2.01049194289390
H	-0.35817172389344	-3.01038547312823	2.75611376344614
H	-0.72232974040915	-1.58441139414878	1.73192995099024

H	-2.05133125049555	-2.50231176491219	2.48943421020204
C	4.62073438646900	-2.91582677760628	1.33864721711631
H	4.41949998247189	-3.89292705875051	1.81168354665992
H	4.98999873512031	-3.08953641512994	0.31504588681386
H	5.42680567084524	-2.42596218021258	1.91265363950965
C	-2.20372085252711	0.58664527759569	-3.80633190446928
H	-1.91254331784723	1.18867370666202	-2.92771281213282
H	-1.74323862276515	1.03975536630826	-4.70135774230727
H	-3.29814573581570	0.66989759255143	-3.92367417109999
C	3.57023981405285	1.67827161853431	-3.71864620608593
H	4.38632477889741	0.95655362892813	-3.89003693144751
H	3.04560559202003	1.84096369352802	-4.67599723745628
H	4.02366933705871	2.64181399017093	-3.42857640396399
C	-2.14683873617023	-1.70846931886100	-4.91514154019188
H	-3.24132595710623	-1.71106984755585	-5.06032680242784
H	-1.68977528861918	-1.27301379858580	-5.82096204288668
H	-1.81869415611161	-2.75734183222603	-4.82472503061641
C	2.81474227281807	-1.82611125695035	2.76874530825464
H	3.55986336562123	-1.30634474560088	3.39586722926189
H	1.88878356485316	-1.22470633231551	2.77815659129170
H	2.60022969947054	-2.79579054445026	3.25059354861345
C	-1.58826766628561	-4.93383092932932	1.10472575789523
H	-2.57905394306626	-4.94574723774543	1.59097692253617
H	-1.64299944701609	-5.56509109803937	0.20231210457483
H	-0.87369163580039	-5.39562736778069	1.80776915980386
C	1.44460203319568	2.18259122810895	-2.39673823869839
H	1.84673088561515	3.13742588197727	-2.01448368872750
H	0.87726581241237	2.39297796945679	-3.31967836423967
H	0.74176164800551	1.79032776973160	-1.63596845927346
H	1.38720265187542	5.51944475386431	3.57060648792385

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97

(DAC*)Cu(CzCN) triplet

Cu	0.02304647770649	0.00014374080877	0.13146964946012
O	3.98033461223424	-2.29531711843158	-2.27099329783123
N	2.10715509840702	-1.38091824808802	-1.29890715472237
N	-0.05950936431148	-2.22104272876601	-1.70109754246959
N	-0.71743821156117	1.39636866766143	1.09415019604113
O	-0.43562642718898	-4.05442560412494	-3.03916374982684
C	-2.06027022779084	1.58635654812405	1.39023626870062
C	0.73120685031059	-1.24928567459359	-1.07530601036506
C	-0.02988011080167	2.44699548714827	1.69855202596453
C	2.96482862611157	-0.39926232418131	-0.65391887397876
N	-7.04870267765377	2.94863087735613	2.94028499544647
C	-2.25505289403892	2.75976890175483	2.19618365796825
C	-0.92368476174205	3.32049383271967	2.39991228102287
C	-0.41686107665599	4.42815386207404	3.08444674813041
H	-1.07959482969873	5.10953813931852	3.62822513508003
C	-1.49100672540404	-2.15161951376985	-1.45530624202407
C	3.59959535208143	-0.73952522794820	0.56729493281694
C	-4.63122812182267	2.30326129689129	2.20180326599202
C	2.74558301240192	-2.31897443455500	-2.11754719721558
C	-4.42538724550537	1.14422911154998	1.40379399292691
H	-5.28742939118542	0.53965254535735	1.11051403643149
C	-3.53693798998173	3.11948294463479	2.60254592157782
H	-3.72127615905950	4.00556995212317	3.21695926039468
C	-3.14217036500943	0.77952878333985	0.99043860127902
H	-2.98325873549216	-0.10964065496994	0.37312416677516
C	-5.95709567808797	2.65657600223009	2.60658844378090
C	1.84743090918690	3.79141785867937	2.37200732778267
H	2.92294349811271	3.99303870755534	2.36948004295690
C	0.97589909222390	4.65605534699181	3.06557006023725
C	1.35788370181869	2.67687236736869	1.67552993966859
H	2.02727016452197	2.01493636255860	1.11781770803678
C	-2.32208939798438	-1.49686950611837	-2.39919884138188
C	1.87812373845325	-3.37067911630797	-2.81641072874571
C	3.19029270449869	0.84157359482890	-1.30164753899283
C	0.37590358856970	-3.25755597117240	-2.53579796258461
C	-2.01701051637092	-2.80000190220681	-0.30975131679541
C	2.48496964006125	1.21558925923988	-2.60222906207229

H	1.98387697865903	0.30844245562457	-2.98196603101908
C	3.41327366227552	-2.10142520899554	1.23184508151713
H	2.58801060887579	-2.61735323440238	0.70953407687792
C	4.46920363520081	0.20876727705423	1.14005918896947
H	4.98156878109474	-0.03242737862527	2.07749667194365
C	-3.71086375122602	-1.50152307872248	-2.16434960720048
H	-4.37671490700345	-1.01267971233168	-2.88349767172826
C	-1.12017266994912	-3.48618990598517	0.71765984866735
H	-0.09918051825218	-3.51984980304894	0.29926522849388
C	-1.76443588850100	-0.84134144493035	-3.65967567501833
H	-0.66374648440197	-0.83248227744674	-3.57118418352252
C	-3.41234612192296	-2.77105130750823	-0.11912513768064
H	-3.84443898336677	-3.26534879946756	0.75762322338715
C	2.35425719797274	-4.77834398732523	-2.35820393436229
H	2.22161658761209	-4.91276436063328	-1.27007776585234
H	1.76414531827850	-5.54978441617730	-2.87784050986205
H	3.42321183141246	-4.89822352138794	-2.59546499812263
C	2.09986514188180	-3.24665488527473	-4.35056065941902
H	1.77195237129481	-2.26091407051956	-4.72526726122929
H	3.17172646858365	-3.36423353152656	-4.57526535201694
H	1.51869368164609	-4.02604516145198	-4.86815955316439
C	4.06782011137138	1.75502768877089	-0.68544720529414
H	4.25898733239884	2.72104982440455	-1.16487679169068
C	-4.25518145084456	-2.13690324697942	-1.04130165819526
H	-5.33982672171660	-2.14198310777126	-0.88631930696255
C	4.70844368076798	1.44161729266041	0.52020913557510
H	5.40112290815247	2.15822078687621	0.97547149905334
C	-1.05953188810390	-2.64102809947090	2.00903304209593
H	-0.35259298668996	-3.07346147545179	2.73885357556386
H	-0.72050822263995	-1.61410195065588	1.76540757274328
H	-2.05029255823410	-2.56088906538765	2.49169420803119
C	4.68718717683524	-2.96153733806739	1.05948308120952
H	4.53000875212549	-3.97222254352760	1.47788427438484
H	4.95072821581364	-3.05480754986160	-0.00650994896561
H	5.54443538502427	-2.50668181669066	1.58866019089456
C	-2.22607802752133	0.62421261339281	-3.80780385708850
H	-1.95271685871277	1.22566079552398	-2.92333888507891
H	-1.75392150529022	1.08325477077182	-4.69464138605757
H	-3.32001628435691	0.69888564662137	-3.94351414959790
C	3.46609482708217	1.69512820476880	-3.69140471350982
H	4.24141986114598	0.93521952484674	-3.88668279092545
H	2.92297449481524	1.88670100158441	-4.63396250332208
H	3.97226474743606	2.63510630801774	-3.40703949257749
C	-2.13050500843258	-1.67567145476549	-4.90920039919741
H	-3.22474525618540	-1.69645846607342	-5.06409286807456
H	-1.67054306083279	-1.23737528315279	-5.81335815776150
H	-1.77812349393772	-2.71402437631093	-4.79871650087166
C	3.01649144471308	-1.98078278726876	2.71846897741986
H	3.81598450548670	-1.51361504675159	3.32109243676192
H	2.10081795958855	-1.37704747588517	2.84685190693417
H	2.82931824108456	-2.98267064109427	3.14428028912879
C	-1.55229418149669	-4.93927927932427	1.00266840033968
H	-2.55159439390247	-4.98865945609839	1.47094999035813
H	-1.58228050597753	-5.53022518747044	0.07186602818644
H	-0.83929778804850	-5.41977970171982	1.69612236657826
C	1.38315033990795	2.2604988962642	-2.31683726514823
H	1.81112264284268	3.20629086152065	-1.93785961603760
H	0.80410965416606	2.48666155778472	-3.22974577669045
H	0.68812439455041	1.86824246363036	-1.55168392546708
H	1.38442259509744	5.52151716397890	3.59698767513193

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98

(MAC*)Cu(CzCN) reduced

Cu	-0.02022382833643	-0.08765673630098	0.07159729553816
N	-2.10714001137720	1.43440700713792	1.28273434274546
O	0.74634284906953	-1.44918805805591	-0.92002951223007
O	-3.96396987997314	2.39958706226316	2.25567806502102
N	0.04276704502643	2.27485688418446	1.59671102346806
C	-0.73590078932089	1.31351100247128	1.06103427684933
C	2.09699680679113	-1.60330714640448	-1.18611966941051

C	0.10421732221158	-2.53125683717496	-1.53053437626752
N	7.17288041854020	-2.86065972616955	-2.60641157247127
C	-2.99037492782225	0.47347953641193	0.62102146029941
C	1.04617184814110	-3.39067610214407	-2.18622877914769
C	-0.77235391028335	-4.82471220442803	-2.88556954290713
C	2.34498826811112	-2.78967875609789	-1.96341533745459
C	0.59841819403383	-4.54023598711277	-2.86312033068314
H	1.31118422379382	-5.20311085392243	-3.36689250970935
C	1.46479023742117	2.32276321950639	1.27323583730377
C	3.16286992645884	-0.76609056600052	-0.79539245298559
H	2.97356790117921	0.14064924911056	-0.21235963887236
C	-0.49508771613859	3.48735773915681	2.24796968081184
H	-0.65068842312232	4.25901443138114	1.46584574213368
H	0.27751281947290	3.87374496886157	2.93439027418249
C	4.45943105206184	-1.10910961965465	-1.17210451070802
H	5.30165489634140	-0.47397646885107	-0.88208982795421
C	3.65175037202154	-3.12558851441160	-2.33613277219618
H	3.86238221311522	-4.02282580785315	-2.92671111795105
C	-3.58766502197814	0.83413947669029	-0.61223935325461
C	6.06143262176954	-2.60458171306866	-2.30778484528065
C	-1.69510608963403	-3.96942323492323	-2.23882912801190
H	-2.76407301324137	-4.20847413187389	-2.27109866736009
C	1.87067333662803	2.98078040431382	0.08293068980655
C	4.71651748711684	-2.28419888373995	-1.93989650857346
C	-3.28483650470121	-0.74733239050847	1.27754698024929
C	2.40131464251579	1.81648391819398	2.21325345244641
C	-1.80855824490163	3.23345818673513	3.00681203959095
C	-1.27251143436036	-2.82078665362446	-1.55890469269547
H	-1.99352985233063	-2.16376779089550	-1.06132729807788
C	-2.74194247279278	2.36652094050332	2.15324305226073
C	3.76942347713189	1.99003467995632	1.93278318293665
H	4.51367336953479	1.59926850009629	2.63308653400126
C	1.95885826191724	1.02050714690056	3.43797202312311
H	0.92134342089778	1.31819463017452	3.66977843286894
C	0.88188422348529	3.44808521538839	-0.98399368421060
H	-0.13739627667847	3.39515082694015	-0.55924092906508
C	-2.63683925738144	-1.15191493696471	2.59983262495106
H	-2.12122052136584	-0.26583771462151	3.01074684841161
C	-4.47858151919696	-0.08495350490710	-1.19827634720297
H	-4.95437872350059	0.16570763660727	-2.15181946963466
C	-1.57112983196452	2.46864920676996	4.33491446862560
H	-1.10176780932025	1.48412082551614	4.17120651543109
H	-2.52992709654636	2.30727735014313	4.85470094555528
H	-0.91174981305492	3.05939901043320	4.99552905890926
C	-3.33914766597009	2.17886405308076	-1.29275352325160
H	-2.49356198928044	2.66919308687407	-0.7765851850373
C	4.19483513489900	2.64818525883352	0.77235897979761
H	5.26449877633087	2.77697332838934	0.57676204816344
C	-2.49026355963336	4.58369038301165	3.30440428537941
H	-2.68009579503497	5.15218785121998	2.37760454378006
H	-1.85036530328130	5.19610058925743	3.96368728466213
H	-3.45759418565068	4.41822213380934	3.80221354715586
C	3.25333739592275	3.12450382804064	-0.14563934135342
C	3.59490514148518	3.61379908847894	-1.06340312304268
H	-4.17821286003083	-1.63088469262997	0.64260852332381
H	-4.41073963317330	-2.58905028514739	1.11832940248230
C	-4.77459773297352	-1.30473155927343	-0.58057752332775
H	-5.47209440182553	-2.00370623061981	-1.05403216306009
C	0.92045868634102	2.46969129204215	-2.18051795121917
H	0.18225059337604	2.75955789214010	-2.94851912230325
H	0.68816808794065	1.44416217706656	-1.83917612250252
H	1.91908801473737	2.44953468844933	-2.65073296979662
C	-1.56007888993876	-2.23138153066330	2.35051726921656
H	-2.00127011080576	-3.15163196417987	1.92949735988952
H	-1.03920263531468	-2.49489663934714	3.28813269444786
H	-0.81094065971459	-1.86038774158320	1.62670433220738
C	1.12145093540687	4.90522159541500	-1.43138931278734
H	2.09560875468573	5.02418682250541	-1.93720303365576
H	1.09950690084699	5.60401531755790	-0.57660705117382
H	0.34114590926714	5.21422276297933	-2.14883563921061

C 1.93546297857192 -0.48677928508615 3.08962134369751
H 1.28772397915341 -0.67724473875736 2.21433062895243
H 1.55678715353933 -1.08068984704165 3.94057733916295
H 2.94786140059516 -0.84862493391528 2.83802122345349
C -4.57475880295093 3.09790452147928 -1.14448509054063
H -4.37150500974156 4.09281545627648 -1.58055266441916
H -4.85117431820830 3.22458580675999 -0.08501507447104
H -5.44553439599603 2.67027040730666 -1.67334837079127
C -3.67070468233681 -1.60459133509828 3.65181492133538
H -4.43662614486738 -0.82846329850138 3.82076149624193
H -3.16734598380023 -1.81192578294060 4.61285958397878
H -4.18752102953903 -2.53165520118983 3.34727346164599
C -2.94151951208251 2.02078808340915 -2.77599663993949
H -3.76658033350531 1.59984673855913 -3.37731830570325
H -2.06720004809115 1.35867378855546 -2.89417195054827
H -2.69274294058575 3.00603491994068 -3.20923039859007
C 2.80836281006264 1.28881071553814 4.69589661102447
H 3.83808362158866 0.90463413058697 4.58933235477901
H 2.36255779152766 0.77544162436339 5.56570550809319
H 2.87048519150955 2.36656052171619 4.92758190801137
H -1.13504884491948 -5.71547373980648 -3.40946804089587

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(MAC*)Cu(CzCN) oxidized

Cu -0.03184084460582 -0.11057066716754 0.01498929406115
N -2.09785043681813 1.41702258760811 1.26393289076212
N 0.70992261505162 -1.47215806038774 -0.99896491075894
O -3.95605669717442 2.39554013625503 2.21842482533757
N 0.05391822061286 2.23914645341602 1.59807866939479
C -0.73831007957847 1.30384431479806 1.05992949273666
C 2.05635582570577 -1.61512105797179 -1.30755523583414
C 0.04523458814349 -2.53470010108499 -1.60395998813834
N 7.07043910425023 -2.81526253037606 -2.88327747082387
C -2.97775028207135 0.45215588322235 0.60069398985036
C 0.96028582715620 -3.38145592856240 -2.31126881428439
C -0.90823562417265 -4.76731878610909 -2.96078043122676
C 2.27988336614291 -2.78097584133005 -2.11519742658085
C 0.48312235877382 -4.50053818249406 -2.99016283358781
H 1.15744860703960 -5.16554202323381 -3.53871169841171
C 1.48372466013135 2.24713350128644 1.29885000286752
C 3.11269825281384 -0.77107991282495 -0.91451523675058
H 2.92562939303800 0.11884483156466 -0.30622311047960
C -0.47103358447279 3.45110085337450 2.27069721768374
H -0.58970323740424 4.23590833225482 1.49662782804152
H 0.29889009471594 3.80484704567640 2.97613411693147
C 4.40607545162823 -1.09772154391864 -1.33094321788335
H 5.25196575286506 -0.46726800897513 -1.04672397351236
C 3.56711799196261 -3.10257479820431 -2.52676811521922
H 3.77882591611966 -3.98187461805719 -3.14145532089392
C -3.58171513772826 0.81483294715191 -0.62952614357473
C 5.97234681473437 -2.56168190245843 -2.54079156165945
C -1.80106577785454 -3.92918845372791 -2.26505720778963
H -2.86981351438039 -4.16119090774951 -2.26182157474504
C 1.92272182593871 2.89422337478469 0.11203271849551
C 4.63937609948162 -2.24984181471791 -2.12804160831228
C -3.26231926755141 -0.77130875933483 1.25979404466290
C 2.39022395867970 1.71689526347268 2.25422073584703
C -1.80448965487700 3.21673776342635 3.00368888976038
C -1.33804694061443 -2.79856437578612 -1.57464980869994
H -2.02426469154746 -2.14692094417128 -1.02476944332431
C -2.73779925974399 2.36435006126060 2.13916585397263
C 3.76749858562895 1.83981590455275 1.98328791734519
H 4.48949473072310 1.43716182538927 2.70112197137774
C 1.93904312232331 1.01352156747419 3.53226520568850
H 0.83615460698962 1.03490885035444 3.55731649612503
C 0.96145488753877 3.41113471410194 -0.95805582084118
H -0.06294537572468 3.39904102736798 -0.54246897609376
C -2.61746036713889 -1.16517190928437 2.58764059378800
H -2.12422585741911 -0.26986040534947 3.00563996693373
C -4.46477035183987 -0.11312872122742 -1.21579298299444

H	-4.95237944715099	0.13888382270917	-2.16273101198435
C	-1.60290485567636	2.45043609863183	4.33848625534601
H	-1.13506853104743	1.46218607797842	4.19165814603975
H	-2.57322777018008	2.29887433169734	4.83852879923633
H	-0.95562879719506	3.04036103332029	5.01070348623309
C	-3.35802474742418	2.16734067609798	-1.30376564495854
H	-2.53195538587839	2.68012246676669	-0.77705263126107
C	4.22777562909825	2.47761753785966	0.82550375076791
H	5.30315766793276	2.57929061370536	0.64623244033874
C	-2.46838629018459	4.58024767852795	3.28713892922810
H	-2.64545640872467	5.14559716074591	2.35624131051894
H	-1.82292020641240	5.18631358956051	3.94594660204751
H	-3.43920655748595	4.43412923606546	3.78385980655078
C	3.31187565137326	2.98817515911665	-0.10250213981472
H	3.68006371514110	3.47710461953061	-1.00993164685871
C	-4.15025967002852	-1.66107387205150	0.62438162222881
H	-4.38826255889307	-2.61455743159729	1.10660204689745
C	-4.75062593686885	-1.33607391209013	-0.59856818277491
H	-5.45486667009561	-2.03280105783895	-1.06522647841470
C	0.96847157052195	2.44187701071015	-2.16231225493503
H	0.23098108902120	2.74893653195095	-2.92325796270367
H	0.71695292943700	1.41824672088031	-1.82497492669536
H	1.96249639993440	2.40298037090219	-2.64123398063544
C	-1.51565378420687	-2.22152899440620	2.34635053112296
H	-1.93945055996708	-3.15918491847125	1.94536124731388
H	-0.97929919397344	-2.46005472703675	3.28113291150844
H	-0.78008337201999	-1.84607058152831	1.60868352709787
C	1.26513325768014	4.85958061852329	-1.39508422561864
H	2.24468308321425	4.94139833045091	-1.89697279988605
H	1.26912277440426	5.55192807406831	-0.53581136508592
H	0.50104129717962	5.20604077960972	-2.11202216561609
C	2.36764689051246	-0.47177161657322	3.53367748334146
H	1.97080639366282	-1.00881536794829	2.65411322265085
H	1.99441383808207	-0.97722792695850	4.44125594139766
H	3.46686810088139	-0.57508711649129	3.52322122810554
C	-4.61952500814618	3.05371931268604	-1.17051269066034
H	-4.43357352655149	4.05332626416315	-1.60157141916243
H	-4.91461909372270	3.17296926369097	-0.11554820164635
H	-5.47179629252421	2.60744350423362	-1.71279980300390
C	-3.64656951939207	-1.64620655522594	3.63162762275733
H	-4.43393792947704	-0.89137045491888	3.79427043271534
H	-3.14535134005523	-1.83784745454779	4.59633372099499
H	-4.13578033931071	-2.58712163641101	3.32542146899623
C	-2.94041311573847	2.02238859005502	-2.78343027072221
H	-3.74615562762646	1.57837410701304	-3.39356582997680
H	-2.04415427977997	1.38795580271060	-2.89718435354130
H	-2.71833407514704	3.01484084791825	-3.21312919213270
C	2.45242236108423	1.73832742070256	4.79689534350981
H	3.55465464394567	1.71809605916281	4.85554877349648
H	2.06276832496066	1.24574597459393	5.70455127780554
H	2.13830449413790	2.79643087313726	4.81869963043355
H	-1.29367884279166	-5.64327514576993	-3.49121849683509

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(MAC*)Cu(CzCN) triplet

Cu	-0.06918245173583	-0.01278164580852	-0.16117313928865
N	-2.11268586187209	1.40767171810302	1.28859098220008
N	0.69895674252151	-1.42895650275081	-1.07182297234119
O	-3.97852593176001	2.28571653365204	2.32793215553947
N	0.06805866378943	2.22092381510411	1.66620082474242
C	-0.74005818108704	1.27178667459373	1.02698483600051
C	2.04907735285495	-1.59578619629853	-1.34911618889913
C	0.04793417877481	-2.53158666908665	-1.62338333480864
N	7.08969927680776	-2.88727737497734	-2.79828391034665
C	-2.98423735531153	0.45678805177805	0.61719708384904
C	0.97295565827172	-3.41375086353374	-2.27122278793453
C	-0.87902347361040	-4.83923212066927	-2.88328426622298
C	2.28495175547729	-2.80403943015824	-2.08994192437716
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H	-0.04308068322296	3.30383080428629	-0.52949838060521
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