

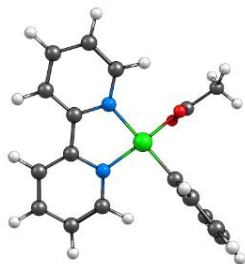
DFT OPTIMIZED STRUCTURES FOR CHAPTER 4: MULTIREFERENCE DESCRIPTION
OF NICKEL–ARYL HOMOLYTIC BOND DISSOCIATION PROCESSES IN
PHOTOREDOX CATALYSIS

Adapted with permission from:

Cagan, D. A.[†]; Strocio, G. D.[†]; Cusumano, A. Q.; Hadt, R. G. Multireference Description of Nickel–Aryl Homolytic Bond Dissociation Processes in Photoredox Catalysis. *J. Phys. Chem. A* **2020**, *124* (48), 9915-9922. <https://doi.org/10.1021/acs.jpca.0c08646>.

[†]Co-first author. *Corresponding author.

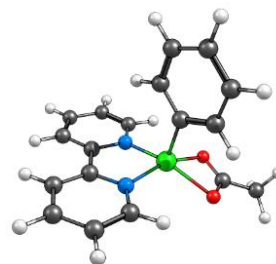
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39

Aryl Carboxylate RKS Fully Optimized

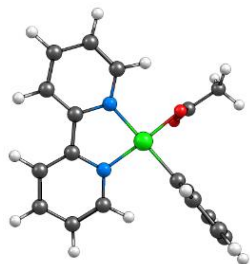
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7	-0.166326000	-1.869074000	-0.070411000
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1	-0.896634000	-5.700614000	-0.447096000
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6	0.190929000	2.451672000	-1.106243000
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1	2.200016000	0.268814000	-2.055522000
1	4.682463000	0.143756000	-1.913297000
1	5.804646000	-0.139214000	0.304678000
1	1.944695000	-0.207871000	2.238925000
1	4.414754000	-0.298307000	2.378800000



39

Aryl Carboxylate Triplet Fully Optimized

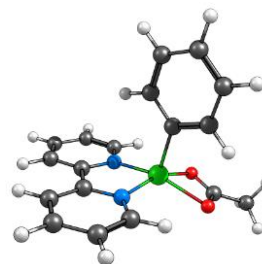
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C	-4.036390125	-0.716285517	-0.828856077
C	-3.827429540	1.689473586	-0.844136718
C	-2.466522118	1.536018327	-0.598002976
N	-1.885355862	0.321777139	-0.473131211
C	-2.655468845	-0.808316711	-0.582965994
C	-1.899132774	-2.055341059	-0.419720306
N	-0.551359209	-1.866233900	-0.239020821
C	-2.451445311	-3.347481997	-0.428190764
H	-4.642029460	-1.621030291	-0.918182042
H	-5.700453833	0.624361759	-1.154767210
H	-4.254050305	2.690045265	-0.943217439
H	-1.786231644	2.385811418	-0.497655678
C	-1.618281973	-4.452618667	-0.267591134
H	-3.527480140	-3.485483993	-0.556753202
C	-0.238083683	-4.246424965	-0.090286737
H	-2.034211972	-5.463163278	-0.274413057
C	0.249010194	-2.943969868	-0.074692325
H	0.449428677	-5.085749941	0.035303239
H	1.308656802	-2.717886913	0.066591713
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	1.941270076
O	0.836868028	1.835220159	-0.459862035
C	1.977186221	1.263314296	-0.559828537
O	2.069773772	0.000000000	-0.379413077
C	3.209901395	2.084526129	-0.855420462
H	2.957051335	2.951952712	-1.480186754
H	3.980962289	1.472020444	-1.341478363
H	3.622881992	2.464069701	0.093678092
C	1.204997611	-0.265392124	2.617918715
C	-1.153541560	0.231472608	2.709904277
C	-1.104433709	0.219800043	4.113437424
C	0.102407966	-0.036987929	4.774486362
C	1.257347547	-0.280109218	4.021031951
H	2.120750551	-0.448127948	2.047164672
H	2.209233659	-0.482775928	4.524868671
H	0.142543927	-0.048147070	5.868267772
H	-2.114785794	0.434005254	2.225455631
H	-2.016591837	0.412088491	4.689700490



39

Aryl Carboxylate RKS 2.0 Å Ni-C distance

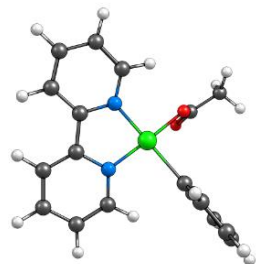
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7	-1.919905000	-0.042136000	0.065034000
6	-2.469004000	-1.294077000	0.018640000
6	-1.454282000	-2.346522000	-0.092158000
7	-0.159670000	-1.864447000	-0.063635000
6	-1.732600000	-3.712503000	-0.211972000
1	-4.275847000	-2.494799000	0.047034000
1	-5.777362000	-0.508728000	0.260458000
1	-4.741255000	1.794336000	0.371448000
1	-2.216058000	1.985699000	0.246974000
6	-0.685062000	-4.629431000	-0.309868000
1	-2.769328000	-4.054693000	-0.236214000
6	0.626916000	-4.141422000	-0.285373000
1	-0.888556000	-5.698538000	-0.406233000
6	0.848774000	-2.771420000	-0.165918000
1	1.485399000	-4.812332000	-0.360653000
1	1.853427000	-2.350398000	-0.145195000
28	0.000000000	0.000000000	0.000000000
6	2.017685000	0.000000000	0.084979000
8	0.052094000	1.865249000	0.070135000
6	0.261577000	2.450291000	-1.097058000
8	0.329276000	1.872299000	-2.184483000
6	0.449054000	3.961064000	-0.977444000
1	-0.018794000	4.370609000	-0.071441000
1	0.054955000	4.459146000	-1.874048000
1	1.529372000	4.173332000	-0.922681000
6	2.806700000	0.141022000	-1.068122000
6	2.648874000	-0.161636000	1.329587000
6	4.050421000	-0.200158000	1.420206000
6	4.833231000	-0.076418000	0.265035000
6	4.208332000	0.097402000	-0.977005000
1	2.325914000	0.312631000	-2.034689000
1	4.812917000	0.209702000	-1.883759000
1	5.925280000	-0.105543000	0.333930000
1	2.055300000	-0.253714000	2.246171000
1	4.529567000	-0.322386000	2.397970000



39

Aryl Carboxylate Triplet 2.0 Å Ni-C distance

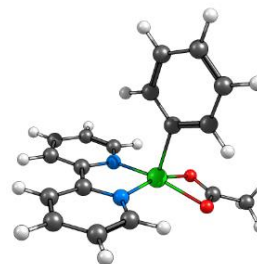
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C	4.057100421	-1.021601326	-0.843960973
C	2.689729649	-1.099243568	-0.598133452
N	1.912595075	0.000000000	-0.473178628
C	2.481802482	1.243488749	-0.582375541
C	1.526490367	2.345598338	-0.419358073
N	0.229634267	1.932361247	-0.239382774
C	1.853706499	3.712207257	-0.427210765
H	4.303699342	2.378801972	-0.916477083
H	5.724444066	0.343521623	-1.153633587
H	4.645958714	-1.936104285	-0.943246646
H	2.161989463	-2.051349421	-0.498170852
C	0.846356613	4.661432164	-0.267123269
H	2.891320837	4.029240368	-0.554737258
C	-0.479645928	4.226007569	-0.091062692
H	1.086525305	5.727512033	-0.273378287
C	-0.740747906	2.860136941	-0.075816723
H	-1.298583365	4.937797875	0.033908133
H	-1.747396249	2.459066739	0.064654992
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.025833398
O	-0.516235484	-1.949939411	-0.459210797
C	-1.736503645	-1.578212110	-0.559195131
O	-2.040268981	-0.348344554	-0.379327501
C	-2.813835266	-2.594882492	-0.854191895
H	-2.419601513	-3.407396504	-1.479472468
H	-3.677155262	-2.120378922	-1.339275366
H	-3.156237996	-3.038468724	0.095266302
C	-1.232470985	0.061798980	2.702298513
C	1.175882678	-0.036629647	2.794683615
C	1.125319354	-0.033305245	4.198219072
C	-0.107531611	0.019487328	4.859078134
C	-1.286691340	0.067585931	4.105440848
H	-2.165779319	0.090001930	2.131454940
H	-2.259113953	0.109418148	4.609077483
H	-0.149116328	0.023721355	5.952855194
H	2.157434700	-0.076313461	2.310253531
H	2.056707289	-0.071442599	4.774543371



39

Aryl Carboxylate RKS 2.2 Å Ni-C distance

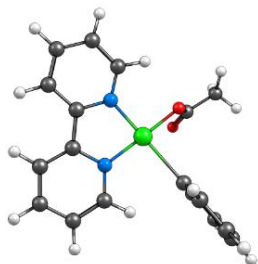
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6	-4.093105000	0.936002000	0.325213000
6	-2.710527000	1.050861000	0.188883000
7	-1.900876000	-0.029012000	0.118851000
6	-2.452735000	-1.279613000	0.203189000
6	-1.443466000	-2.340459000	0.136965000
7	-0.150389000	-1.857802000	0.075468000
6	-1.721836000	-3.711431000	0.131440000
1	-4.256663000	-2.465399000	0.406745000
1	-5.748464000	-0.461773000	0.505220000
1	-4.707209000	1.837899000	0.373320000
1	-2.188234000	2.008557000	0.135640000
6	-0.675153000	-4.631715000	0.054800000
1	-2.757221000	-4.055577000	0.177954000
6	0.634777000	-4.142788000	-0.017480000
1	-0.878170000	-5.705228000	0.047430000
6	0.857419000	-2.767490000	-0.007486000
1	1.491064000	-4.817459000	-0.083340000
1	1.859289000	-2.342582000	-0.060260000
28	0.000000000	0.000000000	0.000000000
6	2.210107000	0.000000000	0.068146000
8	0.074219000	1.860972000	-0.064346000
6	0.332518000	2.353160000	-1.264029000
8	0.422543000	1.692127000	-2.301484000
6	0.550808000	3.864041000	-1.250899000
1	0.037046000	4.353341000	-0.411606000
1	0.226165000	4.297101000	-2.206939000
1	1.630313000	4.058354000	-1.141099000
6	2.971220000	0.113324000	-1.102453000
6	2.850501000	-0.117764000	1.308629000
6	4.254430000	-0.140120000	1.379426000
6	5.017579000	-0.042891000	0.208673000
6	4.375204000	0.086342000	-1.029904000
1	2.471408000	0.249395000	-2.064842000
1	4.967101000	0.176188000	-1.947554000
1	6.110802000	-0.058803000	0.262541000
1	2.268332000	-0.188293000	2.234054000
1	4.750248000	-0.228379000	2.352605000



39

Aryl Carboxylate Triplet 2.2 Å Ni-C distance

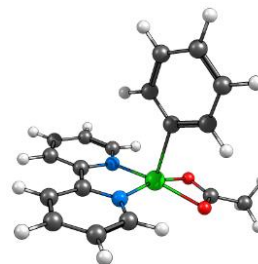
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C	4.088687563	-1.023608091	-0.602009839
C	2.708182227	-1.099817676	-0.438355225
N	1.927429704	0.000000000	-0.348712378
C	2.506212156	1.241182483	-0.409963344
C	1.545042921	2.346652362	-0.281769430
N	0.243903154	1.932936002	-0.152741106
C	1.875141420	3.711355013	-0.268997848
H	4.345938815	2.375557190	-0.624960397
H	5.773901983	0.338615433	-0.802325139
H	4.680267902	-1.938973987	-0.673731656
H	2.173993051	-2.051576885	-0.377266195
C	0.863328261	4.661494134	-0.135677401
H	2.916723004	4.027975884	-0.359574183
C	-0.466899457	4.226694283	-0.009003596
H	1.105200201	5.727152781	-0.125261999
C	-0.730523809	2.860236717	-0.017602335
H	-1.288570248	4.938579947	0.096296870
H	-1.741833015	2.458825699	0.083293418
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.197500429
O	-0.536904347	-1.943675784	-0.430091582
C	-1.758921921	-1.566314538	-0.455967846
O	-2.041940901	-0.331157593	-0.272071153
C	-2.859809208	-2.578310207	-0.666047091
H	-2.522979478	-3.384568968	-1.331940944
H	-3.761474175	-2.098401716	-1.068734024
H	-3.116671995	-3.032993284	0.304858135
C	-1.238215885	0.057306671	2.849842482
C	1.174446651	-0.031449408	2.957346771
C	1.115457604	-0.018213462	4.361872019
C	-0.123663664	0.034419658	5.012111005
C	-1.300896379	0.071949651	4.253877591
H	-2.164770989	0.079591638	2.267185310
H	-2.274962260	0.112345414	4.754810681
H	-0.171681095	0.045570898	6.105699091
H	2.156121867	-0.073288968	2.472046127
H	2.041782018	-0.049648609	4.947045036



39

Aryl Carboxylate RKS 2.4 Å Ni-C distance

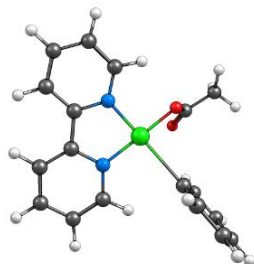
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6	-4.093614000	0.935805000	0.087977000
6	-2.706864000	1.049996000	0.006576000
7	-1.893561000	-0.030042000	0.023002000
6	-2.446630000	-1.278690000	0.141548000
6	-1.433325000	-2.337617000	0.162176000
7	-0.141112000	-1.850691000	0.135718000
6	-1.704594000	-3.709439000	0.196183000
1	-4.255532000	-2.459105000	0.321502000
1	-5.753365000	-0.457696000	0.261950000
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1	-2.183616000	2.005795000	-0.068698000
6	-0.650147000	-4.624377000	0.194686000
1	-2.739135000	-4.058950000	0.213248000
6	0.659410000	-4.130649000	0.154167000
1	-0.847107000	-5.698782000	0.219029000
6	0.875484000	-2.754353000	0.123031000
1	1.520483000	-4.802344000	0.145354000
1	1.875031000	-2.321633000	0.094835000
28	0.000000000	0.000000000	0.000000000
6	2.391834000	0.000000000	0.229742000
8	0.092403000	1.854557000	-0.125019000
6	0.483230000	2.288894000	-1.310912000
8	0.665197000	1.577545000	-2.302402000
6	0.723712000	3.795429000	-1.343664000
1	0.116586000	4.331241000	-0.600578000
1	0.528445000	4.183464000	-2.352641000
1	1.783759000	3.983661000	-1.106960000
6	3.205034000	0.103799000	-0.902325000
6	2.956788000	-0.097039000	1.504587000
6	4.356100000	-0.105794000	1.650303000
6	5.178791000	-0.015907000	0.520046000
6	4.604057000	0.090098000	-0.753643000
1	2.753735000	0.217064000	-1.890967000
1	5.244262000	0.170701000	-1.639257000
1	6.267670000	-0.021476000	0.632613000
1	2.324283000	-0.161514000	2.396650000
1	4.800214000	-0.177361000	2.649599000



39

Aryl Carboxylate Triplet 2.4 Å Ni-C distance

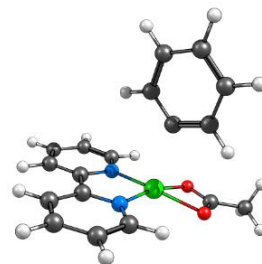
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C	2.7144416756	-1.099405743	-0.363531767
N	1.932270860	0.000000000	-0.282900696
C	2.514161271	1.240425754	-0.315961048
C	1.550360583	2.346604217	-0.196454391
N	0.248057265	1.931468823	-0.092422757
C	1.880954620	3.710196364	-0.166436126
H	4.358728981	2.375669463	-0.471718960
H	5.790053046	0.338926339	-0.632385365
H	4.691922813	-1.938165213	-0.553225397
H	2.178527664	-2.051396355	-0.325731645
C	0.867026105	4.659738637	-0.038592697
H	2.923737043	4.027383520	-0.239350423
C	-0.464208569	4.224095195	0.064057138
H	1.108937233	5.725152221	-0.014117777
C	-0.728217100	2.857462688	0.036243295
H	-1.287163353	4.935042448	0.165853949
H	-1.740878634	2.454988225	0.117565906
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.369167217
O	-0.548099175	-1.939838356	-0.410363773
C	-1.769502225	-1.559543571	-0.395139553
O	-2.041812984	-0.322185199	-0.208296562
C	-2.879745113	-2.569431078	-0.559774334
H	-2.570848400	-3.377414376	-1.237078053
H	-3.795720107	-2.088569473	-0.927445310
H	-3.098639536	-3.022265390	0.421197000
C	-1.243583104	0.052514568	3.004505843
C	1.172430745	-0.028760456	3.126433206
C	1.104443106	-0.013021677	4.531426115
C	-0.139834900	0.036816220	5.172691256
C	-1.314056744	0.069185674	4.408990596
H	-2.165268990	0.071853329	2.413668786
H	-2.290563897	0.106886388	4.905575603
H	-0.194313321	0.049388008	6.265984983
H	2.155411989	-0.068976919	2.643072968
H	2.026649227	-0.040759697	5.123450598



39

Aryl Carboxylate RKS 2.6 Å Ni-C distance

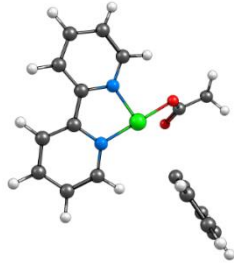
6	-4.650982000	-0.407914000	0.330148000
6	-3.801992000	-1.515781000	0.265619000
6	-4.093534000	0.877183000	0.273942000
6	-2.712136000	1.014349000	0.149994000
7	-1.887326000	-0.054819000	0.074642000
6	-2.421979000	-1.316088000	0.140046000
6	-1.396756000	-2.361123000	0.061803000
7	-0.112354000	-1.855567000	0.025374000
6	-1.648968000	-3.736239000	0.017867000
1	-4.209724000	-2.527661000	0.318729000
1	-5.730593000	-0.545373000	0.427597000
1	-4.720863000	1.769731000	0.326659000
1	-2.202225000	1.979540000	0.111809000
6	-0.582685000	-4.632779000	-0.076133000
1	-2.677631000	-4.102054000	0.046260000
6	0.718589000	-4.118236000	-0.128833000
1	-0.764593000	-5.709476000	-0.112974000
6	0.916090000	-2.739606000	-0.078981000
1	1.587192000	-4.775344000	-0.208724000
1	1.907678000	-2.288387000	-0.110176000
28	0.000000000	0.000000000	0.000000000
6	2.586202000	0.000000000	0.207671000
8	0.078132000	1.858565000	-0.014305000
6	0.487561000	2.352695000	-1.169975000
8	0.697856000	1.687613000	-2.187961000
6	0.722238000	3.859301000	-1.125697000
1	0.083792000	4.358747000	-0.383432000
1	0.563921000	4.291909000	-2.122855000
1	1.771047000	4.040271000	-0.838729000
6	3.363817000	0.259947000	-0.922042000
6	3.179480000	-0.244047000	1.447356000
6	4.582611000	-0.245524000	1.557775000
6	5.374295000	0.000008000	0.428347000
6	4.766601000	0.253680000	-0.808757000
1	2.884231000	0.485808000	-1.877906000
1	5.383020000	0.455729000	-1.691979000
1	6.465617000	0.000474000	0.513975000
1	2.569650000	-0.429853000	2.338076000
1	5.053144000	-0.433244000	2.529639000



39

Aryl Carboxylate Triplet 2.7 Å Ni-C distance

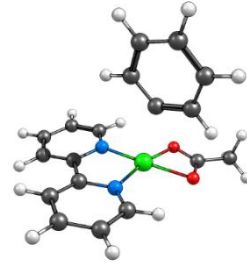
C	4.693846108	0.253460832	-0.554366775
C	3.894627874	1.389045429	-0.406680804
C	4.089200320	-1.012810663	-0.530819618
C	2.707899416	-1.094912239	-0.366321697
N	1.928311319	0.000000000	-0.221828487
C	2.510556160	1.240647729	-0.235761798
C	1.548056697	2.342202156	-0.053801320
N	0.247098920	1.920279003	0.036678933
C	1.879225845	3.701559864	0.035714322
H	4.345658143	2.383799227	-0.425501266
H	5.774062049	0.353410905	-0.686665104
H	4.679710342	-1.925370431	-0.639115323
H	2.173835304	-2.048409509	-0.344781612
C	0.865655277	4.644460143	0.217130977
H	2.921709780	4.021606183	-0.029062563
C	-0.463319506	4.203240627	0.310064103
H	1.107569122	5.707593343	0.290509146
C	-0.728071917	2.838946343	0.217630101
H	-1.285603551	4.907746328	0.453960205
H	-1.739985656	2.432514233	0.286871132
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.712499828
O	-0.562161219	-1.930162793	-0.379252813
C	-1.781587404	-1.554084277	-0.278133807
O	-2.042874622	-0.317621379	-0.072952058
C	-2.896421410	-2.568344358	-0.364656728
H	-2.637305805	-3.368887967	-1.071146270
H	-3.840357075	-2.089350958	-0.655952928
H	-3.035958629	-3.031091487	0.626063913
C	-1.260563817	0.039697057	3.303476211
C	1.160266088	-0.025364584	3.480455571
C	1.058358005	-0.011459771	4.884649038
C	-0.202238258	0.028724381	5.495206525
C	-1.361178330	0.053740684	4.707385664
H	-2.166176973	0.053919817	2.687670735
H	-2.348001623	0.082647960	5.183926839
H	-0.281405115	0.038742472	6.586961699
H	2.151207571	-0.058982002	3.013027861
H	1.965965116	-0.033632154	5.499173690



39

Aryl Carboxylate RKS 2.9 Å Ni-C distance

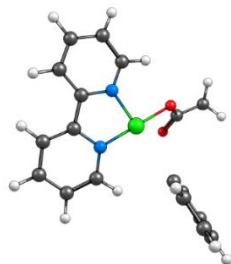
6	4.666210000	0.280284000	-0.003624000
6	3.845413000	1.410286000	-0.045116000
6	4.071357000	-0.990225000	-0.001114000
6	2.682488000	-1.091459000	-0.043028000
7	1.883612000	0.000000000	-0.096503000
6	2.455506000	1.248249000	-0.091074000
6	1.455926000	2.319683000	-0.144812000
7	0.160594000	1.850792000	-0.059783000
6	1.735042000	3.683916000	-0.280374000
1	4.282444000	2.411416000	-0.032863000
1	5.752888000	0.388692000	0.031889000
1	4.676983000	-1.898602000	0.034164000
1	2.145813000	-2.042948000	-0.030428000
6	0.683962000	4.600716000	-0.349135000
1	2.770914000	4.024010000	-0.346598000
6	-0.630492000	4.119151000	-0.289377000
1	0.886689000	5.669108000	-0.455166000
6	-0.854898000	2.751194000	-0.148834000
1	-1.486598000	4.794621000	-0.347873000
1	-1.854756000	2.321769000	-0.079978000
28	0.000000000	0.000000000	0.000000000
6	-2.791804000	0.202148000	0.810161000
8	-0.163798000	-1.861240000	0.060620000
6	-0.893088000	-2.264828000	-0.960505000
8	-1.315485000	-1.508715000	-1.845182000
6	-1.216127000	-3.752148000	-0.940863000
1	-0.404802000	-4.343560000	-0.493181000
1	-1.429859000	-4.104199000	-1.958792000
1	-2.118023000	-3.908451000	-0.326584000
6	-3.768013000	-0.126845000	-0.126357000
6	-3.116466000	0.607300000	2.101567000
6	-4.473462000	0.701657000	2.467215000
6	-5.472624000	0.386515000	1.536940000
6	-5.123217000	-0.027045000	0.244177000
1	-3.483663000	-0.468756000	-1.125062000
1	-5.904182000	-0.280699000	-0.481687000
1	-6.526980000	0.458239000	1.822330000
1	-2.339755000	0.847808000	2.835293000
1	-4.744146000	1.017245000	3.481369000



39

Aryl Carboxylate Triplet 2.9 Å Ni-C distance

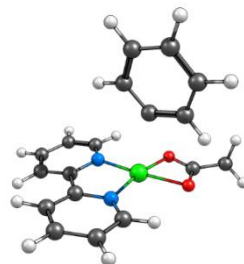
C	4.708041113	0.273931660	-0.098425746
C	3.891006879	1.405125617	-0.037857388
C	4.113807696	-0.997497697	-0.060888739
C	2.726488977	-1.090200246	0.030970616
N	1.929074581	0.000000000	0.106257614
C	2.502416755	1.246809062	0.071940062
C	1.519870742	2.338251388	0.161730674
N	0.222899102	1.909675908	0.026968357
C	1.822419219	3.689649516	0.376537447
H	4.328687279	2.404907755	-0.089903473
H	5.792471500	0.380621473	-0.181873970
H	4.717890851	-1.906799994	-0.100010179
H	2.201686736	-2.048734644	0.054150126
C	0.785782713	4.623034985	0.438527564
H	2.859271871	4.006438448	0.511778993
C	-0.537925845	4.177251443	0.296416270
H	1.003774662	5.680497809	0.606910791
C	-0.775970629	2.818898859	0.103151370
H	-1.377716895	4.874518527	0.337971709
H	-1.783537045	2.409801850	-0.002010183
Ni	0.000000000	0.000000000	0.000000000
C	-0.555032749	0.170577451	2.825112220
O	-0.486998438	-1.939189324	-0.332493792
C	-1.715917447	-1.583732965	-0.410250161
O	-2.013441084	-0.342798596	-0.316840067
C	-2.796047587	-2.624592073	-0.572186231
H	-2.437849693	-3.462764235	-1.185590268
H	-3.700336153	-2.184850000	-1.012865558
H	-3.056458522	-3.025678787	-0.421008082
C	-1.910528960	0.230468112	3.128456223
C	0.426574474	0.203413500	3.807886826
C	0.033540049	0.303608631	5.156830732
C	-1.326691508	0.367684499	5.487963572
C	-2.298535592	0.330643026	4.478601091
H	-2.666260717	0.194662096	2.336741263
H	-3.362432114	0.377333642	4.738487376
H	-1.630334943	0.444548095	6.536771882
H	1.491328250	0.150192609	3.554823550
H	0.793460341	0.329628278	5.946468854



39

Aryl Carboxylate RKS 3.1 Å Ni-C distance

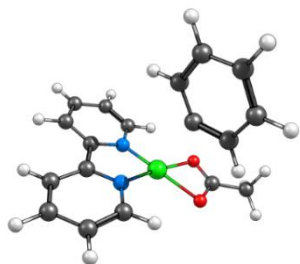
6	-4.619758000	0.605388000	-0.117922000
6	-4.031447000	-0.655821000	-0.188015000
6	-3.789592000	1.745195000	-0.096700000
6	-2.411105000	1.579244000	-0.148861000
7	-1.827577000	0.358106000	-0.255352000
6	-2.634007000	-0.767745000	-0.260532000
6	-1.863336000	-1.998532000	-0.333645000
7	-0.518763000	-1.794315000	-0.081858000
6	-2.355936000	-3.282758000	-0.618016000
1	-4.648607000	-1.557591000	-0.162650000
1	-5.706371000	0.706564000	-0.062780000
1	-4.211344000	2.751591000	-0.047859000
1	-1.715576000	2.421738000	-0.125777000
6	-1.481886000	-4.366584000	-0.643339000
1	-3.417237000	-3.420415000	-0.839597000
6	-0.111892000	-4.144608000	-0.398234000
1	-1.853037000	-5.370817000	-0.862167000
6	0.327118000	-2.852330000	-0.135333000
1	0.604914000	-4.968463000	-0.398996000
1	1.374753000	-2.617468000	0.063810000
28	0.000000000	0.000000000	0.000000000
6	0.540181000	-0.773187000	2.997753000
8	0.779251000	1.799592000	0.112648000
6	1.950554000	1.271857000	0.085397000
8	2.027061000	0.000000000	-0.030295000
6	3.179691000	2.126783000	0.224800000
1	3.024041000	3.105668000	-0.249101000
1	4.053711000	1.624522000	-0.210124000
1	3.376993000	2.300537000	1.295258000
6	1.872979000	-1.027322000	3.285811000
6	-0.469986000	-0.831069000	3.944907000
6	-0.120624000	-1.163142000	5.269002000
6	1.216674000	-1.425857000	5.596723000
6	2.212446000	-1.359427000	4.612522000
1	2.642589000	-0.970185000	2.509473000
1	3.257034000	-1.565212000	4.872565000
1	1.484485000	-1.683713000	6.626008000
1	-1.514384000	-0.625078000	3.686752000
1	-0.896633000	-1.215647000	6.041076000



39

Aryl Carboxylate Triplet 3.1 Å Ni-C distance

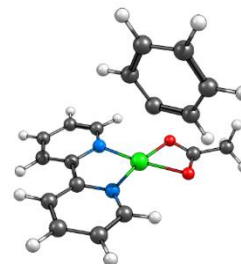
C	4.668911097	0.278251076	-0.429837405
C	3.858299803	1.408116680	-0.302925651
C	4.080818908	-0.994433766	-0.335491836
C	2.707940989	-1.089380945	-0.121376855
N	1.917119386	0.000000000	0.026456249
C	2.485671567	1.249532558	-0.066792678
C	1.511182616	2.333989366	0.099864848
N	0.208817057	1.900299921	0.016192761
C	1.817254965	3.681636413	0.333117036
H	4.284936440	2.409057082	-0.404644737
H	5.741194246	0.385298437	-0.611473500
H	4.680643299	-1.903287410	-0.422230115
H	2.189551330	-2.048901676	-0.049368054
C	0.781075129	4.607311878	0.468015400
H	2.858637338	3.998291998	0.429577106
C	-0.546923935	4.156663945	0.382754841
H	1.002011876	5.661647464	0.651477712
C	-0.788838137	2.802344362	0.170175671
H	-1.386793431	4.848106461	0.481052541
H	-1.798831417	2.390690178	0.106492804
Ni	0.000000000	0.000000000	0.000000000
C	-0.494358589	0.204258580	3.008654402
O	-0.496911519	-1.938756313	-0.253165834
C	-1.729583400	-1.588666604	-0.238780212
O	-2.018169879	-0.345251393	-0.139118418
C	-2.817382683	-2.630884557	-0.302242405
H	-2.502908618	-3.481620780	-0.922173744
H	-3.750061797	-2.198620291	-0.687810204
H	-3.008515956	-3.010862936	0.714699689
C	-1.847151113	0.254104628	3.315733664
C	0.501541073	0.252216291	3.973282430
C	0.119308393	0.359045062	5.325053451
C	-1.238693167	0.413309488	5.668064735
C	-2.221311587	0.360636224	4.669589742
H	-2.606812819	0.207140774	2.528624495
H	-3.282459534	0.400718981	4.940946701
H	-1.532455929	0.495002918	6.719177940
H	1.562923661	0.206285415	3.706425883
H	0.885521482	0.398109997	6.107812395



39

Aryl Carboxylate RKS 3.3 Å Ni-C distance

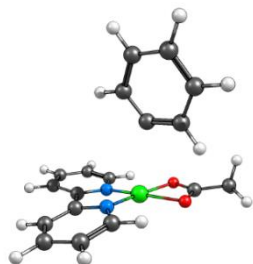
6	-4.625000000	0.562765000	0.051717000
6	-4.026528000	-0.695595000	0.063932000
6	-3.807704000	1.705940000	-0.067091000
6	-2.431214000	1.545359000	-0.170083000
7	-1.839731000	0.324054000	-0.197669000
6	-2.632969000	-0.803844000	-0.066449000
6	-1.853321000	-2.030858000	-0.072076000
7	-0.501013000	-1.797194000	0.106991000
6	-2.344375000	-3.336801000	-0.231943000
1	-4.631521000	-1.595976000	0.198370000
1	-5.708851000	0.660698000	0.150401000
1	-4.237910000	2.709737000	-0.087204000
1	-1.745011000	2.391666000	-0.254276000
6	-1.461853000	-4.413931000	-0.206554000
1	-3.412391000	-3.498337000	-0.398728000
6	-0.085037000	-4.163832000	-0.038981000
1	-1.831920000	-5.434896000	-0.328310000
6	0.351847000	-2.851583000	0.099761000
1	0.639190000	-4.980452000	-0.003364000
1	1.405133000	-2.595135000	0.232760000
28	0.000000000	0.000000000	0.000000000
6	0.760439000	-0.600966000	3.169206000
8	0.775545000	1.807903000	-0.072512000
6	1.945155000	1.278084000	-0.074996000
8	2.020293000	0.000000000	-0.069412000
6	3.178260000	2.138763000	-0.048674000
1	3.009298000	3.071037000	-0.604739000
1	4.039255000	1.596688000	-0.461291000
1	3.407188000	2.408010000	0.995416000
6	2.120674000	-0.803808000	3.339963000
6	-0.160225000	-0.619634000	4.203261000
6	0.320216000	-0.858469000	5.506518000
6	1.689377000	-1.068597000	5.722295000
6	2.588986000	-1.042346000	4.647757000
1	2.811113000	-0.777914000	2.491364000
1	3.658361000	-1.206794000	4.821627000
1	2.057994000	-1.253754000	6.735843000
1	-1.228890000	-0.454642000	4.029779000
1	-0.379286000	-0.879596000	6.349722000



39

Aryl Carboxylate Triplet 3.3 Å Ni-C distance

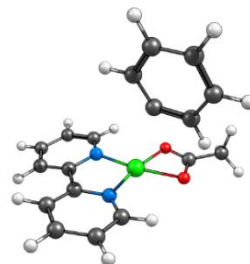
C	4.670889835	0.222555601	-0.200245452
C	3.864546315	1.361288400	-0.230724850
C	4.066648314	-1.033067011	-0.006783851
C	2.685193482	-1.101961081	0.147290364
N	1.895501881	0.000000000	0.149667621
C	2.480413805	1.233892890	-0.046532731
C	1.506805874	2.326019874	-0.042924389
N	0.208933885	1.880662566	-0.176769225
C	1.798293215	3.691091766	0.088091007
H	4.302145813	2.345242975	-0.417543605
H	5.751543759	0.306191878	-0.339428407
H	4.662250857	-1.948048644	0.031174123
H	2.156920610	-2.047939864	0.290666549
C	0.758249907	4.621143914	0.068686326
H	2.831740487	4.017927295	0.227876834
C	-0.563705313	4.159055750	-0.061661156
H	0.968676985	5.688624515	0.170178520
C	-0.794684526	2.790909838	-0.165517736
H	-1.406344432	4.853746676	-0.084105371
H	-1.799592215	2.372184108	-0.257980841
Ni	0.000000000	0.000000000	0.000000000
C	-0.827411399	0.598328092	3.152074776
O	-0.499113179	-1.949105488	-0.012773436
C	-1.727920785	-1.591883589	-0.063627676
O	-2.000884357	-0.340858548	-0.123879601
C	-2.827709608	-2.621033818	-0.017483553
H	-2.505819670	-3.553512585	-0.500716807
H	-3.740205694	-2.237412250	-0.492694577
H	-3.059621512	-2.851063096	1.035332109
C	-2.209503257	0.656477212	3.231298769
C	0.018644803	0.774233852	4.234045867
C	-0.566838328	1.031362824	5.490073602
C	-1.961337802	1.100622365	5.613416917
C	-2.782648931	0.914306839	4.492566681
H	-2.836553314	0.504560775	2.347092021
H	-3.872396001	0.967307947	4.594460334
H	-2.411351552	1.299581198	6.590871428
H	1.107418877	0.716884875	4.132496251
H	0.071249047	1.175780298	6.369103775



39

Aryl Carboxylate RKS 3.5 Å Ni-C distance

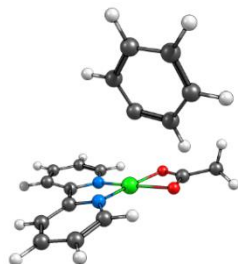
6	4.645576000	0.259662000	0.245650000
6	3.836933000	1.393445000	0.192582000
6	4.046048000	-1.011518000	0.131735000
6	2.668364000	-1.097119000	-0.030833000
7	1.874724000	0.000000000	-0.121961000
6	2.453228000	1.252334000	0.003080000
6	1.473252000	2.323796000	-0.078208000
7	0.175899000	1.863544000	0.067638000
6	1.738063000	3.687832000	-0.280988000
1	4.269021000	2.389149000	0.321947000
1	5.724365000	0.355895000	0.390820000
1	4.644947000	-1.924535000	0.161045000
1	2.144672000	-2.052642000	-0.114572000
6	0.682507000	4.595347000	-0.332024000
1	2.767905000	4.025542000	-0.422391000
6	-0.636128000	4.114930000	-0.199010000
1	0.875111000	5.659686000	-0.487624000
6	-0.844726000	2.752876000	-0.017008000
1	-1.491712000	4.793281000	-0.223386000
1	-1.842679000	2.322882000	0.091571000
28	0.000000000	0.000000000	0.000000000
6	-1.099418000	0.670088000	3.239062000
8	-0.452621000	-1.926063000	-0.027049000
6	-1.693237000	-1.600773000	-0.046667000
8	-1.983967000	-0.353197000	-0.072708000
6	-2.766216000	-2.654478000	-0.003886000
1	-2.432082000	-3.565642000	-0.518470000
1	-3.696306000	-2.280413000	-0.451796000
1	-2.971401000	-2.917887000	1.046631000
6	-2.480650000	0.575247000	3.247163000
6	-0.327254000	0.944646000	4.353675000
6	-0.997894000	1.139214000	5.578267000
6	-2.395773000	1.052682000	5.634600000
6	-3.137684000	0.772646000	4.478469000
1	-3.042237000	0.354281000	2.334376000
1	-4.230194000	0.705980000	4.528515000
1	-2.911218000	1.204491000	6.587778000
1	0.764540000	1.010726000	4.302403000
1	-0.422881000	1.358268000	6.484817000



39

Aryl Carboxylate Triplet 3.6 Å Ni-C distance

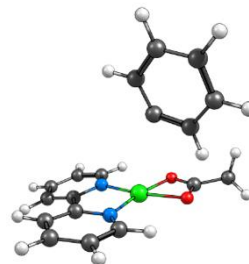
C	4.652768551	0.248397312	-0.340308909
C	3.844348193	1.384346398	-0.291098731
C	4.056010899	-1.017748235	-0.188400369
C	2.680981863	-1.098426156	0.006559091
N	1.889506431	0.000000000	0.090243210
C	2.466676537	1.245415306	-0.068265333
C	1.490686728	2.328463802	0.015191924
N	0.190431415	1.879190971	-0.108025901
C	1.774946151	3.688674627	0.204214770
H	4.273535274	2.377472573	-0.446862566
H	5.728179127	0.341563962	-0.510518556
H	4.653805962	-1.931776864	-0.212841503
H	2.159462256	-2.052004881	0.121377657
C	0.728959238	4.610104282	0.255784325
H	2.809627417	4.016166868	0.333744938
C	-0.593868297	4.143920900	0.138280876
H	0.934752869	5.673240262	0.402467468
C	-0.818671440	2.780963536	-0.024417271
H	-1.441457156	4.832247736	0.169085135
H	-1.822806747	2.359333431	-0.111945636
Ni	0.000000000	0.000000000	0.000000000
C	-0.958525837	0.555630482	3.394605993
O	-0.493288420	-1.946969499	-0.041814946
C	-1.722734606	-1.591566987	-0.024026769
O	-1.995573962	-0.337878068	-0.025062245
C	-2.821231450	-2.621045711	0.031076683
H	-2.513744385	-3.542616875	-0.481278729
H	-3.745970422	-2.226694062	-0.410734826
H	-3.025829650	-2.873278137	1.084505712
C	-2.339967841	0.540560425	3.315709519
C	-0.236297733	0.748748954	4.557901817
C	-0.967026090	0.946824568	5.747253016
C	-2.368478467	0.942022744	5.719262229
C	-3.055379404	0.740333254	4.513806999
H	-2.855978941	0.378154408	2.364567865
H	-4.150868868	0.736367142	4.499061578
H	-2.930262786	1.095705050	6.645529823
H	0.858377461	0.749729106	4.570890777
H	-0.435222239	1.103616092	6.692116013



39

Aryl Carboxylate RKS 3.9 Å Ni-C distance

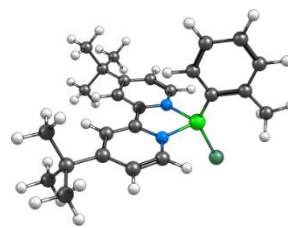
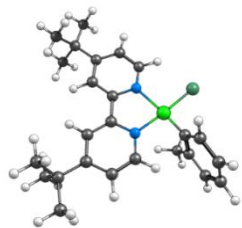
6	4.649472000	0.268464000	-0.147066000
6	3.835596000	1.400251000	-0.153230000
6	4.045524000	-1.004537000	-0.194105000
6	2.659207000	-1.094012000	-0.246026000
7	1.857052000	0.000000000	-0.291001000
6	2.442088000	1.254015000	-0.231427000
6	1.456494000	2.324626000	-0.254932000
7	0.177646000	1.869764000	0.020589000
6	1.701443000	3.679904000	-0.525362000
1	4.273426000	2.398640000	-0.072418000
1	5.736094000	0.368317000	-0.088445000
1	4.646862000	-1.916519000	-0.199126000
1	2.133501000	-2.051757000	-0.273989000
6	0.644967000	4.588719000	-0.511225000
1	2.714300000	4.009963000	-0.770408000
6	-0.656025000	4.115144000	-0.247927000
1	0.822126000	5.647069000	-0.717837000
6	-0.846683000	2.759447000	-0.006248000
1	-1.510790000	4.794559000	-0.218285000
1	-1.832072000	2.335790000	0.199934000
28	0.000000000	0.000000000	0.000000000
6	-1.182382000	0.981031000	3.631192000
8	-0.465793000	-1.940456000	0.062378000
6	-1.691780000	-1.600820000	0.202940000
8	-1.974950000	-0.348972000	0.207517000
6	-2.765113000	-2.639904000	0.391508000
1	-2.480509000	-3.581671000	-0.096284000
1	-3.726159000	-2.280779000	-0.000593000
1	-2.890310000	-2.840109000	1.468322000
6	-2.521353000	0.749570000	3.378649000
6	-0.653448000	1.399147000	4.836718000
6	-1.562529000	1.605922000	5.894759000
6	-2.932907000	1.387498000	5.695937000
6	-3.414049000	0.962691000	4.449508000
1	-2.871093000	0.415812000	2.397245000
1	-4.486219000	0.793757000	4.301899000
1	-3.632772000	1.549742000	6.521015000
1	0.418672000	1.566719000	4.979788000
1	-1.192502000	1.937493000	6.870871000



39

Aryl Carboxylate Triplet 3.9 Å Ni-C distance

C	4.642398146	0.223090009	-0.430936682
C	3.836647745	1.361508339	-0.420590304
C	4.045651306	-1.034121482	-0.212243978
C	2.674287626	-1.102935541	0.008578636
N	1.885324276	0.000000000	0.056940036
C	2.462197041	1.236710429	-0.169357432
C	1.488669968	2.321687944	-0.121323889
N	0.185833521	1.865589278	-0.206406549
C	1.772605490	3.689894391	0.001236675
H	4.264288314	2.345547151	-0.629578526
H	5.714997354	0.305791571	-0.622910380
H	4.641509833	-1.949727903	-0.204596740
H	2.153616179	-2.049356902	0.174928284
C	0.726359862	4.611826943	0.023198699
H	2.808433847	4.023808159	0.102651312
C	-0.598101136	4.139389829	-0.054772135
H	0.932472402	5.680840466	0.117328490
C	-0.823406409	2.770491855	-0.149793159
H	-1.446069576	4.827900122	-0.046222020
H	-1.828160829	2.344870187	-0.204963158
Ni	0.000000000	0.000000000	0.000000000
C	-1.291392700	0.874636817	3.589988220
O	-0.493454408	-1.944005330	0.087694750
C	-1.721415157	-1.585688514	0.112105687
O	-1.992777151	-0.333114310	0.046365205
C	-2.821570882	-2.605892205	0.248266375
H	-2.511805746	-3.568997173	-0.178822119
H	-3.741739997	-2.250589874	-0.234753823
H	-3.038031296	-2.762939061	1.317753686
C	-2.623713155	0.771037899	3.237858390
C	-0.814425609	1.205534585	4.843611682
C	-1.773007898	1.459612783	5.845945433
C	-3.139615569	1.370743696	5.547249787
C	-3.566163855	1.029679019	4.255998107
H	-2.948715122	0.501630599	2.227968346
H	-4.636252121	0.961744571	4.031305374
H	-3.879474331	1.568494630	6.328607838
H	0.255696618	1.271112725	5.063938275
H	-1.444695546	1.725626454	6.856478643



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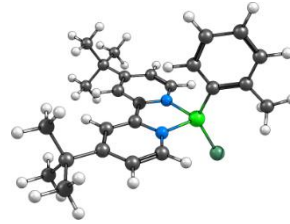
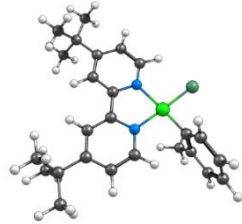
Aryl Chloride RKS 1.6 Å Ni-C distance

Ni	-0.00009519129503	-0.00016310960331	-0.00000559617899
C	-2.43145763719745	1.41863184932317	0.01090148403728
C	-2.79218288280194	-0.87955592552047	0.08630258146515
C	-3.80984294345521	1.64694475770289	0.04767053979983
C	-4.17205284067798	-0.70011716425471	0.12147756022553
H	-2.35431376070488	-1.87764533291615	0.10513647032714
C	-4.73205874349013	0.58928814213786	0.10340561047272
H	-4.16752313526241	2.67855463662640	0.03529119683099
H	-4.79821914686812	-1.59238178530806	0.16475167365093
C	-1.42168697925816	2.48616110132030	-0.04585755681574
C	-1.70183475889974	3.85653736721692	-0.10297702777062
C	-0.66374388074989	4.80317804644603	-0.14851345937532
H	-2.74145120316643	4.19012588392263	-0.11482155355137
C	0.85965547017024	2.91122269938295	-0.07769745091348
C	0.64473960934390	4.28895882008757	-0.13279348990369
H	1.86328949382268	2.47703457827532	-0.06691450042889
H	1.51428075555177	4.94679422047674	-0.16408375840904
C	-0.00009559771166	-1.60016300372786	-0.00058392471423
C	-0.12221385815623	-2.34862869860776	-1.21119290609299
C	-0.02330951103334	-2.31748115982147	1.22218853849375
C	-0.30809684522590	-3.74052661513035	-1.14825106454678
C	-0.21094514897102	-3.70634074695283	1.26135279573674
C	-0.36716174035979	-4.42613516656720	0.07198310463159
H	-0.40256666639296	-4.29987850124645	-2.08708388831807
H	-0.22554242021213	-4.22238145923508	2.22753073214437
Cl	2.16958162235690	-0.00533808857864	0.00036995323203
N	-1.90267773774330	0.14473981132651	0.02915552834309
N	-0.14244973411924	2.01368476715378	-0.03497032567136
H	0.11914945114475	-1.78042729741296	2.16632049421215
H	-0.51105147672642	-5.51066297610340	0.08947739439966
C	-6.24241363233700	0.86328281810150	0.14350559355303
C	-0.98104397731519	6.30557436382766	-0.21179879772830
C	-6.65310736158452	1.64611110658773	-1.12863322216664
H	-6.42777959660785	1.07086453742722	-2.04044926365421
H	-6.13272552705455	2.6135838823135	-1.20557741884427
H	-7.73580092532322	1.85235855088687	-1.11541877387570
C	-6.57463823214545	1.70848102526103	1.39859199209978
H	-6.05188683452903	2.67770441439613	1.39535070233297
H	-6.29228040572331	1.17853194678159	2.32189153445182
H	-7.65641088186042	1.91539837519315	1.44236327985018
C	-7.06375736480908	-0.43956315058676	0.20114818309673
H	-6.83797349226754	-1.03118155574553	1.10270746584361
H	-6.89182825981827	-1.07627899792377	-0.68138920814884
H	-8.13831067456971	-0.20010631938629	0.22758389708582
C	-1.81257129857104	6.59738874071479	-1.48578652492613
H	-2.76676946792446	6.04791216281599	-1.49316369714698
H	-1.25829245052479	6.31898698793331	-2.39591709347576
H	-2.04854575641794	7.67226980241051	-1.54690519961388
C	-1.79830773566687	6.70640281992162	1.04159626203189
H	-1.23344728030796	6.50752878855141	1.96597062913101
H	-2.75181103054882	6.15950145412295	1.10713803466336
H	-2.03463666097684	7.78254616573156	1.01245904754398
C	0.29694692164003	7.16583755620177	-0.25627521722561
H	0.91210110492095	6.94734411777658	-1.14371175771337
H	0.92194273492345	7.02540584573261	0.64004590327677
H	0.02472404851955	8.23192113195889	-0.30135425892844
C	-0.02321235292252	-1.66271102502664	-2.55757282274326
H	0.95405575968638	-1.16489895884798	-2.67051430214195
H	-0.79216515308397	-0.88021816194102	-2.68457314132458
H	-0.13755440471084	-2.38009037652062	-3.38597216361538

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Aryl Chloride Triplet 1.6 Å Ni-C distance

Ni	-0.00001814851899	0.00024948128067	0.00016081043439
C	2.41995753548792	1.23118368271145	-0.83123144085451
C	2.72318443713820	-1.06426620841106	-0.51181974512951
C	3.78669336670465	1.38424319001933	-1.10624220215431
C	4.08144323859412	-0.96887805059321	-0.79701034713428
H	2.25537413550443	-2.02087875664166	-0.26586902783566
C	4.65691523790333	0.28423741190075	-1.10031750859210
H	4.17144864340233	2.38112035823472	-1.33331715853182
H	4.68070967563701	-1.87983332511796	-0.77898330925812
C	1.42511935719793	2.31126840525159	-0.83103341905930
C	1.68965401396902	3.66083304569517	-1.10620004557063
C	0.66472681773066	4.61835012135148	-1.09997884185452
H	2.71463552836385	3.96247971488487	-1.33381310645378
C	-0.83759823043493	2.80176560168237	-0.51078499098607
C	-0.63122565212074	4.14763052019311	-0.79599325010892
H	-1.82928539195277	2.41398423526266	-0.26455829225082
H	-1.48996997283918	4.81956246443707	-0.77769292888122
C	-0.00006088900496	-0.00017432515758	1.60016075158076
C	-0.90679192783471	-0.83531661143128	2.34877100417521
C	0.88107234251476	0.81100793382467	2.36910616821349
C	-0.87440810973496	-0.80581789680791	3.757080844445163
C	0.89737383101644	0.82569883925765	3.7659690032336
C	0.00876463373093	0.00731579354513	3.7659690032336
H	-1.57317871109478	-1.44945664361412	4.30458082312950
H	1.60171250797638	1.47411765804728	4.29854679471734
Cl	-1.21044418570149	-1.11448980214495	-1.54589838988431
N	1.89734865248229	0.00023746476285	-0.52955664390824
N	0.15555158594843	1.89137691241157	-0.52898120920058
H	1.592202033119444	1.46573239857858	1.84863364019347
H	0.00138983942653	0.00027213230947	5.56611428530248
C	6.15101468615610	0.46948007169922	-1.41196794250195
C	0.92173945626243	6.09216036616715	-2.92403342295449
C	6.30602433441343	1.06749472148547	-2.83250359176511
H	5.86859018024529	0.40326508007517	-3.59435934215682
H	5.81663309060162	2.04964427075511	-2.92403342295449
H	7.37292149440754	1.20509961897815	-3.07282950710634
C	6.77235539750064	1.43667419332219	-0.37366800631592
H	6.29487093048741	2.42870541604546	-0.39464701222559
H	6.67488014777875	1.03950694129191	0.64901844433448
H	7.84514993263563	1.58052024099371	-0.58209189010635
C	6.92343517563573	-0.86332171649925	-1.35848139249800
H	6.87769043924177	-1.32874681956528	-0.36087509932960
H	6.54736284900771	-1.58968791017796	-2.09661672119393
H	7.98577103263421	-0.68534073307491	-1.58747320338789
C	1.57882677251139	6.19733496395498	-2.83338846740993
H	2.51733565450395	5.62889504119388	-2.92595486630029
H	0.88001233225945	5.81589540720696	-3.59440212555015
H	1.80336981995968	7.24928305181999	-3.07410354197176
C	1.98795032500450	6.63201628368602	-0.37510950463238
H	1.58530233440629	6.56771715623104	0.64805619922923
H	2.93731783031230	6.07452682144358	-0.39711789001919
H	2.21931190588506	7.68930918549521	-0.58397820185112
C	-0.29297780067161	6.97153347294900	-1.35737628951425
H	-1.04863261453991	6.65631779439354	-2.09460527928443
H	-0.75945320979732	6.96438540690526	-0.35923480079919
H	-0.02848829494889	8.01558745897346	-1.58686492836864
C	-1.90939070172314	-1.75870668442517	1.68554935274587
H	-2.61254087206837	-1.21656051298995	1.03430570972460
H	-1.42677019618432	-2.50409449124866	1.03444514537944
H	-2.49786780560347	-2.30060704680800	2.44208719346150



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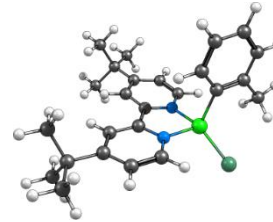
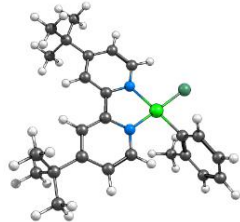
Aryl Chloride RKS 1.8 Å Ni-C distance

Ni	-0.00002879528857	-0.00005290828175	0.00010736647551
C	-2.39732076031478	1.41830539624174	0.01579002381288
C	-2.78090063746139	-0.87846025090131	-0.00294303125105
C	-3.77308044035989	1.66049095560419	0.02233782756931
C	-4.15928055119254	-0.68396970490465	0.00124695488195
H	-2.35259623868496	-1.88058167322444	-0.00903770104575
C	-4.70672148167320	0.61117873413428	0.01472863461740
H	-4.11927543741318	2.69621445380687	0.03411271391587
H	-4.79513731565527	-1.57043133400755	-0.00559127275680
C	-1.37135685819065	2.46868182264374	0.02268378669924
C	-1.62172029279259	3.84504172596520	0.03234581561764
C	-0.56454975649523	4.77155620040930	0.04043904910092
H	-2.65494447684533	4.19846580379019	0.03314418973405
C	0.92161313887808	2.84732882005648	0.02829000412507
C	0.73293989886166	4.22935955743009	0.03852919547093
H	1.91616269847368	2.39295319142558	0.02569438357458
H	1.61605274152883	4.86961657846533	0.04458823289850
C	-0.00000964811992	-1.80005288154110	-0.00019906341853
C	-0.06110545865039	-2.54045624138021	-1.20741773904902
C	-0.06117034121954	-2.49056479802610	1.22511725899322
C	-0.21098306236977	-3.93834062450885	-1.14476842806771
C	-0.20829792839914	-3.88544966896525	1.27061124077580
C	-0.29331757066434	-4.61391842704291	0.07946585048811
H	-0.25651576931811	-4.50819413884838	-2.08068464280682
H	-0.25003231089645	-4.39763189154562	2.23785056991832
Cl	2.16490389913508	-0.08137803512117	0.00018634022254
N	-1.87907591282569	0.13781091561163	0.00315253216250
N	-0.09951922712769	1.96822219672867	0.02018076917060
H	0.02203228724412	-1.93638918476868	2.16634372430243
H	-0.40616768753580	-5.70232938152234	0.09982178453405
C	-6.21493710219446	0.89935243067356	0.02230360694704
C	-0.85048101731024	6.28131277302125	0.05120697731763
C	-6.58235106861198	1.73171251041252	-1.23149980467300
H	-6.33686151885389	1.18731101005884	-2.15695006527983
H	-6.05079299562125	2.69578348553296	-1.25884990187736
H	-7.66298942675060	1.94879296316273	-1.24096162533981
C	-6.57476385991447	1.70222752293214	1.29737263533236
H	-6.04261664092379	2.66524449355646	1.34410688475097
H	-6.32396062931439	1.13629199442869	2.20835438837251
H	-7.65526853850058	1.91922896302613	1.31827115975833
C	-7.04988947929149	-0.39606831784487	0.00959942734061
H	-6.85513230686808	-1.02229917381229	0.89488840648992
H	-6.85910738700478	-1.00211332489085	-0.89049536578464
H	-8.12248105306619	-0.14659596355366	0.01486976275361
C	-1.66770603363355	6.65427989105091	-1.21078750322422
H	-2.63285276018884	6.12565838395015	-1.25093429919195
H	-1.11339827906562	6.41055269271002	-2.13079893862843
H	-1.88139515563435	7.73552815748045	-1.21891386688970
C	-1.66728934498775	6.63574565180392	1.31882933393902
H	-1.11260499313612	6.37870800825399	2.23497907670478
H	-2.63226450216062	6.10627707439292	1.35157444874394
H	-1.88118880003508	7.71672492750265	1.34282239650962
C	0.44530513489964	7.11571120490022	0.05700252743125
H	1.06162734976338	6.92911942907415	-0.83690237886884
H	1.06136514632763	6.91734223103630	0.94853749296922
H	0.19558157445829	8.188222319000452	0.06411301320013
C	0.06331837431322	-1.85007190304765	-2.54799550253367
H	1.03417863560046	-1.33430881552447	-2.62906512263754
H	-0.71548719806888	-1.08054467895890	-2.68974203373523
H	-0.01566962375261	-2.56495128305577	-3.38244373656241

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Aryl Chloride Triplet 1.8 Å Ni-C distance

Ni	-0.00006183850344	0.00024711447285	0.00001133050884
C	2.44024470402626	1.22355589042359	-0.77226673773056
C	2.73111674208350	-1.06725417322856	-0.43137553311302
C	3.80522826954629	1.36823504012220	-1.05399847346495
C	4.09132205694173	-0.98072511921332	-0.71443326551062
H	2.25948909808227	-2.01913729514657	-0.17459192278445
C	4.67155071593231	0.26382671534331	-1.03548247047599
H	4.19403299123585	2.36049218707771	-1.29365741824276
H	4.68742999671712	-1.89335498080987	-0.68040212045696
C	1.45056142817960	2.31271774305159	-0.77213352901019
C	1.72487818203026	3.65766524009005	-1.05380589597672
C	0.70827169565455	4.62552597535164	-1.03495876113198
H	2.74968772338891	3.94990252903756	-1.29374435637438
C	-0.80190739572664	2.82101075957172	-0.43067369978277
C	-0.58592115942905	4.16677626343574	-0.71357691668393
H	-1.79443289654528	2.44243112992562	-0.17372693622958
H	-1.43744898788985	4.84729094122924	-0.67926272421595
C	-0.00014909714491	-0.00005227196299	1.80001130286397
C	-0.89659980639900	-0.81475297161792	2.55438334639711
C	0.89694504740106	0.81493890478811	2.52539741699421
C	-0.85172438572350	-0.77411889272742	3.96202535223915
C	0.93306115482571	0.84756623855019	3.92513270088251
C	0.04874224784062	0.04400576703272	4.65156404827941
H	-1.54661970554407	-1.40564741437365	4.52844441331419
H	1.64805008168858	1.49712146926642	4.44209532754983
Cl	-1.24546001245444	-1.13177326274131	-1.46176173818456
N	1.90995550153085	0.00022630377906	-0.46086236743909
N	0.18223971222379	1.90163158026701	-0.46053751640797
H	1.60289430321331	1.4564580222791	-1.35162916794198
H	0.05745705097425	0.05178391043647	5.74615847090916
C	6.16560132737820	0.43884367019327	-1.35211204926111
C	1.02512852695281	0.09606223890002	1.98206344186459
C	6.31988369259030	1.01577498454604	-2.78144889591104
H	5.87917964212969	0.34201448677489	-3.53298471156927
H	5.83374763899965	1.99820087935146	-2.88646680076304
H	7.38681349256427	1.14628042840080	-3.02531703100417
C	6.79187468316309	1.41877136531359	-0.32876959823823
H	6.31831414682301	2.41229747340861	-0.36346013990230
H	6.69461047591251	1.03691761719856	0.69971771556380
H	7.86479355173248	1.55541565546284	-0.54101944145874
C	6.93296848884858	-0.89596731974394	-1.28056482286522
H	6.88748397075661	-1.34656256936111	-0.27617571303283
H	6.55284428342061	-1.63159613526717	-2.00736987914345
H	7.99549558165485	-0.72535246481566	-1.51404814658409
C	1.61328651860416	6.19459686204678	-2.78129659012769
H	2.54463868485065	5.61671999967429	-2.88693521182939
H	0.89999742567418	5.82046819927039	-3.53244858915214
H	1.84513051979310	7.24416711931180	-3.02519959701200
C	2.06112950990159	6.62563194909790	-0.32891588566016
H	1.67241529118712	6.56523174983047	-1.27923961564910
H	3.00477989607566	6.05921167317627	-0.36431507150456
H	2.29962722186481	7.68058616600918	-0.54121105595587
C	-0.23008389756955	6.98760318051929	-1.2923961564910
H	-0.99915949700804	6.67965508583302	-2.00558654188438
H	-0.68232817105357	6.98538840977913	-0.27456127560633
H	0.04129838307982	8.02893378242890	-1.51284372387608
C	-1.90380424051790	-1.73019249815296	1.88906086606668
H	-2.59935335355294	-1.17838260668677	1.23721234779066
H	-1.42067635403350	-2.47542102589422	1.23759662483967
H	-2.50143465337890	-2.27307739626479	2.63803678533353



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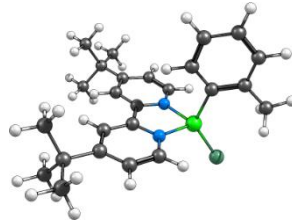
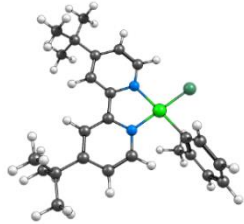
Aryl Chloride RKS Fully Optimized

Ni	1.25914263866544	-1.29757372487669	-0.14112525437629
C	-0.53174202130060	0.822736263138977	-0.05276765965357
C	1.66882229381741	1.58482149937974	-0.09475688098736
C	-1.00041811644866	2.13755601376627	-0.01594938200899
C	1.24638321690200	2.91079811341753	-0.05677506044416
H	2.72774103352657	1.32971435780501	-0.13107327951978
C	-0.12169966702071	3.23352499929650	-0.01636271773084
H	-2.07925406113239	2.30512352686027	0.01374107432126
H	2.01391709480731	3.68608976935289	-0.06033122930693
C	-1.39263143480114	-0.36642486475297	-0.05295364225741
C	-2.79074638678948	-0.35569668576642	-0.01574421366813
C	-3.52334485816867	-1.55557176679547	-0.02061400682915
H	-3.31453146242078	0.60196657867422	0.01773258177511
C	-1.37443268109171	-2.69117663415023	-0.10054220131032
C	-2.76780579930842	-2.74084937248017	-0.06487415953652
H	-0.75731215719097	-3.59314116075665	-0.13480541898368
H	-3.24785264820125	-3.27032346798859	-0.07211723022273
C	3.12167799417186	-0.98525023074852	-0.21289635542658
C	3.88713966266663	-0.84006451036810	0.96707410642455
C	3.73442935142503	-0.78892449449916	-1.46139520337966
C	5.24206114585184	-0.47418450938750	0.85633735540310
C	5.08769209787184	-0.42730317983252	-1.55596047625282
C	5.84336057278074	-0.26077583456522	-0.39062653672574
H	5.83796598690090	-0.36284189962233	1.77020551289907
H	5.54677431674462	-0.28304535751910	-2.53982302287140
Cl	1.72076309007112	-3.41224871316937	-0.19215085325278
N	0.81734183325104	0.52585068203240	-0.09374530448884
N	-0.68231175198931	-1.53458309165407	-0.09506518765389
H	3.17563893991219	-0.93357642425723	-2.38121911477150
H	6.89988598270750	0.01894601327378	-0.44922887060878
C	-0.65734502626263	4.67204552570972	0.02450604903262
C	-5.05921626916135	-1.53232244816780	0.02036859476526
C	-1.49469553694754	4.86914370827726	1.31285159728213
H	-0.88484449529059	4.69914097904711	2.21411461062482
H	-2.35520170679103	4.18334406818115	1.35630102700777
H	-1.88824327947235	5.89779649575126	1.35739925369609
C	-1.55320168785508	4.91876094207600	-1.21503149159144
H	-2.41524944149532	4.23419170433869	-1.24560349843737
H	-0.98577866310069	4.78494194026435	-2.14948079092735
H	-1.94763424698216	5.94795307964326	-1.20086016146429
C	0.48051932323975	5.71159325100046	0.01864066976738
H	1.09909773993250	5.64243184315293	-0.89043370459579
H	1.14096453079650	5.60657776911028	0.89422305831025
H	0.05588365268223	6.72720953839913	0.04896934929135
C	-5.52387743589316	-0.81303922857806	1.31123275116574
H	-5.16680567530302	0.22757305102885	1.35733578111832
H	-5.15835532455597	-1.33312100462607	2.21066792518388
H	-6.62484696915958	-0.78800634997499	1.35671367346684
C	-5.59021531154789	-0.76660623867138	-1.21713818715370
H	-5.27289080024962	-1.25302899077683	-2.15296073101891
H	-5.23486465871328	0.27528739372898	-1.24373330169090
H	-6.69203617921610	-0.74088870301986	-1.20389692229145
C	-5.65991034716769	-2.95161252088294	0.01016972473181
H	-5.34110698622560	-3.54215257144896	0.88387603002167
H	-5.38917654798001	-3.50913605271111	-0.90064927672812
H	-6.75893994070766	-2.88927610549583	0.04085694122440
C	3.27652035100237	-1.10068026789563	2.32611105203635
H	2.91963209269041	-2.14124019976414	2.39589697590361
H	2.40209888798489	-0.45384149149462	2.51466279390370
H	4.00137774553978	-0.93107637825930	3.13807883881008

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Aryl Chloride Triplet Fully Optimized

Ni	-0.23540777135903	0.310184446026536	0.13459255983897
C	2.29083220390681	1.34518716335624	-0.591071766611350
C	2.41894178782609	-0.95941701734680	-0.25254800890352
C	3.67862265222037	1.40681453530990	-0.77180375522411
C	3.79551904156790	-0.95610423959661	-0.44849690163390
H	1.88527657974779	-1.88410687668948	-0.01892292753061
C	4.47396337289971	0.25251156758757	-0.71426446802925
H	4.14289137231177	2.37915759083879	-0.95208714706508
H	4.32971735121659	-1.90484279452097	-0.38444273600487
C	1.38209920467270	2.49849260938635	-0.63322982142253
C	1.74031281367590	3.80991529531082	-0.97339327091469
C	0.79120954430733	4.84434481210330	-0.96910637049882
H	2.77527271715399	4.02080757817278	-1.25200158271982
C	-0.83262578609093	3.16770319808593	-0.28797819363013
C	-0.52576622945333	4.48674680618784	-0.60996933761666
H	-1.84507684647038	2.85345034800304	-0.02328745335014
H	-1.32674288603741	5.22628783262283	-0.58093048412576
C	-0.00426178361110	0.03714090469346	2.04627432835091
C	-0.34056591998319	-1.20678524282082	2.63175418766855
C	0.50687966242832	1.05698112348022	2.86358650884769
C	-0.16578561154844	-1.37757882343230	4.01850902790557
C	0.66858535963986	0.87839459568668	4.24660042341246
C	0.32968658980627	-0.34762781558011	4.82664292113218
H	-0.42894601153568	-2.34097653800853	4.47196327789024
H	1.05973915161548	1.69510656527290	4.86323368198969
Cl	-2.29838784081982	-0.05305797102294	-0.53980969461748
N	1.65736749083207	0.15399977748992	-0.32945459299786
N	0.09150037144065	2.18567235375279	-0.29926766590483
H	0.78326605897266	2.02334074500650	2.0237268559753
H	0.45344245570863	-0.50655411562674	5.90253052610902
C	5.99500307552973	0.33854120901088	-0.91730410703323
C	1.19915668901311	6.27752324448861	-1.3738072779932
C	6.29212938093399	0.93777174673205	-2.31444038628769
H	5.86971382619168	0.31055726178903	-3.11532007825794
H	5.87572618815676	1.95086322895679	-2.42745052436924
H	7.38036832994346	1.00736067340604	-2.47519715448153
C	6.60372146201723	1.25167435246038	0.17613215913840
H	6.19728418621283	2.27421413254278	0.13429841238705
H	6.40471099864452	0.85357102548860	1.18349088805518
H	7.69616942960706	1.32315793809600	0.04739670325123
C	6.66971524315749	-1.04438094113250	-0.82787951857095
H	6.52602650002621	-1.51214043038746	0.15922973123088
H	6.29483174932957	-1.73829436734654	-1.59735783938977
H	7.75464638879000	-0.93844340051619	-0.98396827282538
C	1.74869187991611	6.28533669297192	-2.79575727092863
H	2.63387251644871	5.63979377123149	-2.90649865716876
H	0.98820308806235	9.53691558667562	-3.51218558099945
H	2.04505921823988	7.30705903133254	-3.08422344743124
C	2.30005538547534	6.76887038900993	-0.37466135160884
H	1.94000784538702	6.77137308892836	0.66625635952401
H	3.20140723071409	6.13773556583065	-0.41603169383638
H	2.60337413407765	7.79682795560992	-0.63192425499973
C	0.01140567702712	7.25697007617969	-1.27227142158854
H	-0.79774873045797	6.98076211464726	-1.96704654621960
H	-0.41110615459666	7.31830032807505	-0.25659273320957
H	0.34755060988619	8.26869912956233	-1.54808054264051
C	-0.90722348730093	-2.34152433496148	1.80382343379753
H	-1.92109958077136	-2.10460881984998	1.44365189768880
H	-0.30747087102689	-2.53984410050117	0.89816971590410
H	-0.95539868367601	-3.27974277629868	2.37860755822987



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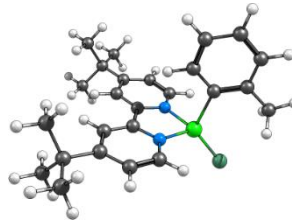
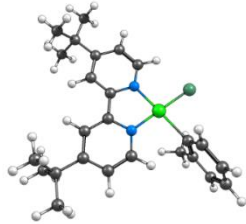
Aryl Chloride RKS 2.0 Å Ni–C distance

Ni	0.0000469694548	-0.00009997227649	0.00087217079841
C	-2.37760056884335	1.41727920835087	0.01773232853815
C	-2.77045973186884	-0.87895611815654	-0.03519455150432
C	-3.75164586504257	1.66630688281888	0.01378225958158
C	-4.14802011858258	-0.67684586400380	-0.04210753505676
H	-2.34435367830657	-1.88198883543815	-0.04947991261306
C	-4.68957198592140	0.62078025041478	-0.01681548112567
H	-4.09301128117879	2.70361935192857	0.03466341987198
H	-4.78822158910819	-1.55986265289561	-0.06704145623046
C	-1.34240882756277	2.45699801839454	0.04701564162629
C	-1.57503680927772	3.83543448094200	0.07832831773572
C	-0.50670812082467	4.74901521768178	0.10567464750656
H	-2.60435587144616	4.20038056378347	0.08155604705070
C	0.95781436255680	2.80737560068764	0.06748327481835
C	0.78412875630896	4.19071891629386	0.09958917615859
H	1.94666467673261	2.34078361264146	0.06128315280620
H	1.67488947235841	4.82004990089809	0.11936454055136
C	-0.00001632789204	-2.00009972232385	-0.00012979488640
C	-0.02012885614027	-2.72290456895650	-1.21111623172477
C	-0.07031331302220	-2.67921623913860	1.22354825203490
C	-0.13857273033766	-4.12519338483461	-1.15579829520696
C	-0.18457049710683	-4.07863670098201	1.26295875178739
C	-0.22616645059369	-4.80303165833842	0.06697044767034
H	-0.15325907518946	-4.69507203686280	-2.09262289348246
H	-0.23429303812089	-4.59641807121572	2.22678944586630
Cl	2.15946269551495	-0.13562291729621	0.00192944783325
N	-1.86504529162909	0.13398157600531	-0.00589892432436
H	-0.07471894124208	1.94068174232352	0.04114911303554
H	-0.02094998035739	-2.12067177556297	2.16424666079796
H	-0.31272351160995	-5.89403779965295	0.08283715528318
C	-6.19656040501340	0.91566661570710	-0.02089649842996
C	-0.77425963948047	6.26166625030509	1.10407349899052
C	-6.547554626667185	1.76519890358627	-1.26789652145739
H	-6.29508242788228	1.23120312314034	-2.19752338874683
H	-6.01141853024581	2.72706117102001	-1.27785985127522
H	-7.62705868839458	1.98738037171525	-1.28560182594258
C	-6.56595654801316	1.70429102516051	1.26031634598015
H	-6.03002292830702	2.66420073339927	1.32449482961533
H	-6.32707494522342	1.12594033750005	2.16669623410137
H	-7.64562928399987	1.92603917370448	1.27286954984035
C	-7.03709791074747	-0.37564443115816	-0.05822955565903
H	-6.85394849326599	-1.01387905006622	0.82095640074659
H	-6.84010968602928	-0.97115538265904	-0.96400707253740
H	-8.10856956834404	-0.12136389431913	-0.06041944514725
C	-1.58149672993214	6.66566995496951	-1.11841274042813
H	-2.55276758065917	6.14950637082931	-1.17132805376676
H	-1.02622931192040	6.43057173776585	-2.04008983302800
H	-1.78215482823594	7.74941693141233	-1.10935213402922
C	-1.59209900462414	6.60520049152552	1.41045126588311
H	-1.04449582930668	6.32628923262757	2.32445782221568
H	-2.56356618128382	6.08707851673134	1.43050585035732
H	-1.79300543293403	7.68817147777077	1.451485482210153
C	0.53162786905479	7.07979828861942	0.16544411062333
H	1.14938439447017	6.90057763354312	-0.72898438423247
H	1.14142235291085	6.85891434960803	1.05599503288331
H	0.29509696673774	8.15505263010846	0.18953930797021
C	0.11060594781991	-2.01626206115483	-2.54134945277335
H	1.07117311143668	-1.47879321163403	-2.59911321840509
H	-0.68227971354287	-1.26161650169875	-2.68322763964503
H	0.05948744441564	-2.72161115428897	-3.38588191600260

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Aryl Chloride Triplet 2.0 Å Ni–C distance

Ni	-0.00034345668129	0.00061355447811	0.00023063429619
C	2.46889925532005	1.22622156571255	-0.63755907947922
C	2.73694470220438	-1.07171742048560	-0.33176538577725
C	3.84185611060566	1.36845734018708	-0.87621244344759
C	4.10628936918074	-0.98709089276282	-0.56810402871228
H	2.25309056655512	-2.02557566408600	-0.10694158705557
C	4.70211696811821	0.25906108680401	-0.85049820151775
H	4.24276325416537	2.36277805232745	-1.08539927449304
H	4.69701519833842	-1.90299554129494	-0.52844575365048
C	1.48574345882195	2.32251586272661	-0.63722751856977
C	1.77601214753516	3.67198839555794	-0.8758839555794
C	0.76649371205768	4.64753896369734	-0.84948566793619
H	2.80788403782996	3.96263545637884	-1.08533242751625
C	-0.76943925545692	2.83821561182004	-0.33059106156386
C	-0.53684126958926	4.19034560346113	-0.56671690018516
H	-1.77010127931126	2.46065437584866	-0.10558147949599
H	-1.38326775018183	4.87689716445868	-0.52670279927419
C	-0.00036773057894	0.00019495810425	2.00023059148485
C	-0.89320151114610	-0.80211789094444	2.75417914189026
C	0.90988101996382	0.81792585575549	2.69057202563583
C	-0.83627355207572	-0.75104856432642	4.16156962575124
C	0.95943715992983	0.86234528740107	4.09198438072261
C	0.07724861643232	0.06970073411054	0.06970073411054
H	-1.52831053495726	-1.37292788670870	4.74219854651241
H	1.68233412227004	1.51180474537954	4.59817439076373
Cl	-1.30486227471549	-1.16970514647242	-1.33871712310754
N	1.92147850125752	0.00037703947582	-0.36818953705231
N	0.20783495526861	1.91124928766682	-0.36754732735489
H	1.61169432667180	1.4485484979526	-0.12967032362519
H	0.09742227918919	0.08774696271767	5.92682910533528
C	6.20597516544790	0.43153004467523	-1.11784426432686
C	1.10096314605058	6.12384788627173	-1.11692313917671
C	6.40708467666430	1.03065694865497	-2.53216248026817
H	5.98748692165207	0.37101862353937	-3.30794278961013
H	5.92845177855140	2.01685871570700	-2.63636249566594
H	7.48161635240493	1.16024796411433	-2.74050300858386
C	6.80462295214590	1.39170138022171	-0.05980659972644
H	6.33746789727781	2.38829551529126	-0.09341353907108
H	6.67319546494444	0.99419066594537	0.95887635697578
H	7.88432270998841	1.52576531028102	-0.23619584628374
C	6.96455105745324	-0.90815997182948	-1.04419510101232
H	6.88596778877119	-1.37446200659692	-0.04907432252493
H	6.60370939103466	-1.63015791368050	-1.79414303033638
H	8.03456023338107	-0.73929472584114	-1.24199915836250
C	1.71798590268913	6.25874105782502	-2.53137463346237
H	2.64641622428714	5.67593491365420	-2.63577860780096
H	1.01652331318851	5.91317170545532	-3.30697474499591
H	1.96334376067193	7.31286136153684	-2.73980654474624
C	2.12070458814878	6.61482806014828	-0.05919113791306
H	1.71158098026539	6.52732668602134	0.95961330500214
H	3.06072196835149	6.04231853739409	-0.09306570288031
H	2.37105750448878	7.67361012352097	-0.23567567150538
C	-0.14847439018856	7.02330887196733	-1.04296853626584
H	-0.90557771360754	6.74291668876392	-1.79269600142796
H	-0.62026261814014	6.99585444497601	-0.47770795819183
H	0.13547601411606	8.06865648685857	-1.24091757564795
C	-1.90516122525292	-1.71163646889006	2.09072340378993
H	-2.59495351022885	-1.15280144413252	1.43862975900805
H	-1.42275805800774	-2.45737223132255	1.43918888782730
H	-2.50788307457110	-2.25289203181426	2.83693885835794



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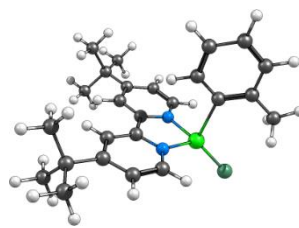
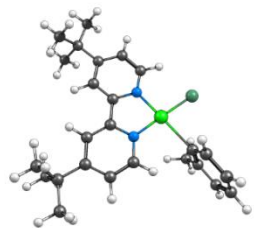
Aryl Chloride RKS 2.2 Å Ni-C distance

Ni	-0.00020430810608	-0.00010885143142	0.00011653007981
C	-2.36772706803534	1.41263124766689	0.01912876933990
C	-2.76111593049140	-0.88493750859964	-0.05032336420421
C	-3.74124272797367	1.66280831310891	0.01126848322988
C	-4.13863867340359	-0.68097197142210	-0.06111314447446
H	-2.33257052172348	-1.88700267695247	-0.06881045425665
C	-4.67909380605197	0.61712553728032	-0.02949708119960
H	-4.08234245904608	2.70018386940789	0.03686830502007
H	-4.77981696338199	-1.56300979200671	-0.09403478024051
C	-1.32807316595997	2.44737451243816	0.05829530537055
C	-1.55144717020819	3.82657274076674	0.09980129930583
C	-0.47741191879499	4.73348817946649	0.13502834403719
H	-2.57879530154462	4.19724922105167	0.10504845122070
C	0.9766889372058	2.78346334705273	0.08360476919629
C	0.81009950567699	4.16724491444783	0.12588822046629
H	1.96245091636072	2.31031921030274	0.07497042275438
H	1.70456379692338	4.79113521140960	0.15120680302216
C	-0.00019858601387	-2.20010881363469	-0.00027780484087
C	0.02368602566605	-2.90062864832187	-1.21841124447639
C	-0.07948882212016	-2.87638944878257	1.21903565338916
C	-0.06462879613247	-4.30644058427257	-1.17578814110347
C	-0.16285434223405	-4.27952627922173	1.24473466932703
C	-0.16099481719940	-4.99323872761875	0.041559254442569
H	-0.04708682973703	-4.87066189833880	-2.11600690510610
H	-0.22145573899502	-4.80728788281421	2.20267101445465
Cl	2.15489840318190	-0.17341036069633	0.00014531984164
N	-1.85696284510281	0.12882801739125	-0.01057747742215
N	-0.06194192691582	1.92357028186996	0.04974257157127
H	-0.06386375823417	-2.3203393583180	2.16200077995777
H	-0.22258842604427	-0.08607815453633	0.04787778485372
C	-6.18601865664888	0.91273463240833	-0.03754544597209
C	-0.7357597129019	6.24738448757765	0.18101755651746
H	-6.53189614657673	1.76963567756176	-1.28094249274186
H	-6.27614682123619	1.24089961606071	-2.21267671976453
H	-5.99530009855900	2.73128590720645	-1.28331649151164
H	-7.61122021420637	1.99243468682339	-1.30145108152572
C	-6.55995039064366	1.69409738462972	1.24680051006596
H	-6.023882746523417	2.65338917420857	1.31860029789622
H	-6.32479846089185	1.11039391985988	2.15072283287042
H	-7.63955846054900	1.91627611502677	1.25651822004426
C	-7.02706421778727	-0.37788180466004	-0.08553463799605
H	-6.84748150695536	-1.02138739107574	0.79054545510732
H	-6.82715802739621	-0.96815942690543	-0.99409544207151
H	-8.09837989116456	-0.12300004685966	-0.09011655416417
C	-1.53911724301471	6.66591051729423	-1.07563013542105
H	-2.51344974377215	6.15607013888060	-1.13349856791976
H	-0.98426159727594	6.43441941157960	-1.99846650956637
H	-1.73324547148998	7.75075522380032	-1.05857298254270
C	-1.55290485019419	6.58647097340481	1.45265014220476
H	-1.00803215181008	6.29740349129348	2.36512877063263
H	-2.52754163828376	6.07415178862869	1.46780196838381
H	-1.74730533673210	7.67030704550074	1.50156543165430
C	0.57509695633606	7.05725927656733	0.21354878106577
H	1.19269343268100	6.88107599456010	-0.68159699423144
H	1.18257136324975	6.82585762167482	1.10301749933517
H	0.34515512614717	8.13373431043382	0.24559141132828
C	0.16546178495899	-2.17294970471088	-2.53509492134431
H	1.11490524036746	-1.61401691696514	-2.56391543448657
H	-0.64074252932657	-1.43314949556858	-2.67875740081148
H	0.14575902330843	-2.86550222641551	-3.39135720457467

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Aryl Chloride Triplet 2.2 Å Ni-C distance

Ni	-0.00168795236911	0.00147877474143	0.00013145350349
C	2.49494127830570	1.23123909595727	-0.46611288519532
C	2.73803566586097	-1.07694924705991	-0.22304323376706
C	3.87750929250232	1.37258650537521	-0.63939500192906
C	4.11719840346384	-0.99280204897540	-0.39280778351405
H	2.24028564021506	-2.03456181353572	-0.05040240285972
C	4.73080333325739	0.25776622866245	-0.61007787957303
H	4.29202425047218	2.37068504945669	-0.79805477818693
H	4.70157534774466	-1.91277387546175	-0.35317013015462
C	1.51781189372609	2.33324064466647	-0.46568368052562
C	1.82359350085115	3.68903675497000	-0.63842627263545
C	0.81898102169825	4.66969570665970	-0.60799148290531
H	2.86409559017251	3.98100396371527	-0.79763587526572
C	-0.74451848771279	2.85078870616602	-0.22119351690247
C	-0.49591596735824	4.21006792363452	-0.39019218659948
H	-1.75475396583176	2.47121562839374	-0.04817049502835
H	-1.33930766309124	4.90030880052190	-0.34957223244601
C	-0.00112220095476	0.00213657754503	2.20013127996893
C	-0.89090629288884	-0.79447380455247	2.95103781187666
C	0.91779654937010	0.82475202005497	2.86043123069020
C	-0.82311423491192	-0.73329786863918	4.35834946791964
C	0.97716431498702	0.87826875583359	4.26298576375457
C	0.09836028572337	0.09189183594528	5.01398924427996
H	-1.51114442692586	-1.34916974604554	4.95025085590437
H	1.70453577514805	1.52948937565452	4.76065469065897
Cl	-1.37084111733222	-1.21391037454054	-1.19356072275829
N	1.92898552066891	0.00051107494337	-0.26297293736519
N	0.22825834189649	1.91854005559606	-0.26227582578802
H	1.61440740821495	1.44806490969696	2.28525807946997
H	0.12725642968584	0.11812044672931	6.10812117043808
C	6.24590987024988	0.42961607284328	-0.80392830109858
C	1.17075745381967	6.15347449814441	-0.81347613077700
C	6.51351901775196	1.07133634457926	-2.18826072952574
H	6.12732401764716	0.43826751760637	-3.00260139831901
H	6.04379213052935	2.06274619625509	-2.28317301259105
H	7.59689759036659	1.20180458193798	-2.34347144096902
C	6.80044186147002	1.35287381193022	0.30957375916273
H	6.34000125965751	2.35287855814674	0.28603148699012
H	6.62096646254770	0.92481810985568	1.30832780362692
H	7.88765662991181	1.48570814114367	0.18642525765940
C	6.99432956553235	-0.91616460152955	-0.73818106729149
H	6.86890148314642	-1.41253308310407	0.23739206954676
H	6.66422172487590	-1.61246331606148	-1.52568670148469
H	8.07291165488142	-0.74766489642556	-0.88249098527603
C	1.83884248421010	6.34294219064965	-2.18602404389163
H	2.76689940027003	5.75804496185942	-2.28178128236494
H	1.16355202498415	6.03549619807940	-2.99989643718103
H	2.09783677592056	7.40299183505412	-2.34107718887731
C	2.15452357178347	6.59303295190917	0.31165443178314
H	1.70888568775140	6.46535948668777	1.31068277891435
H	3.09234700770605	6.01647872574201	0.28698927463783
H	2.41617475054597	7.65667390537057	0.18895777813243
C	-0.07569304804324	7.05758058966448	-0.73422528806294
H	-0.80719881352772	6.81359659205673	-1.52119637182112
H	-0.58265945525858	6.99218922943577	0.24176927786530
H	0.22066580090798	8.10827264932158	-0.87839143640168
C	-1.90457898485349	-1.70292706969298	2.29114026061002
H	-2.59139966395365	-1.14129733262553	1.63844292250098
H	-1.42093763731604	-2.44825640411581	1.64013637934471
H	-2.50849022510289	-2.24289075280037	3.03735738139344



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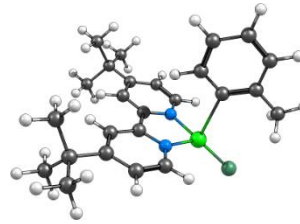
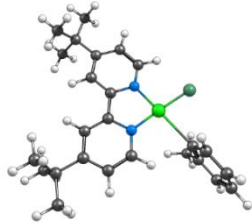
Aryl Chloride RKS 2.4 Å Ni-C distance

Ni	-0.00009344637744	-0.00001549369818	-0.00062395488460
C	-2.36523535235569	1.40251409358776	0.01921321855469
C	-2.75178095078939	-0.89756081985090	-0.06621698969251
C	-3.73916839247594	1.64920447172649	0.00693148646056
C	-4.12986701681762	-0.69641081721943	-0.08161921108961
H	-2.31739680060980	-1.89717427450826	-0.08835434959737
C	-4.67341759840319	0.60039556548713	-0.04437644852338
H	-4.08365012633806	2.68538718583475	0.03704117720456
H	-4.76909042454337	-1.57951081982065	-0.12258782505535
C	-1.32530070916455	2.43676691508216	0.06889452853653
C	-1.54654226578502	3.81560758102072	0.12120476613187
C	-0.47143068990345	4.72112938930102	0.16524312934315
H	-2.57366773608930	4.18704720289218	0.12840439069675
C	0.98176602996038	2.77020827676579	0.09993644100097
C	0.81559794741930	4.15357287524885	0.15304887384201
H	1.96682417081038	2.29560760545681	0.08888430837985
H	1.71060574387759	4.77643308598882	0.18451755431201
C	-0.00001335664635	-2.40001543592967	-0.00010695345305
C	0.08002914720689	-3.07478813888479	-1.22590654443555
C	-0.10206270469905	-3.08034544922630	1.21109807313674
C	0.02089859740762	-4.48332545331324	-1.20084828463160
C	-0.15557320181468	-4.48635625172908	1.21779596137902
C	-0.09823678060139	-5.18421116133575	0.00669444199970
H	0.08016416121932	-5.03731049088852	-2.14550603221887
H	-0.23356685563548	-5.02716525633020	2.16710646638534
Cl	2.15188210200149	-0.19706988246690	-0.00143360257312
N	-1.85236149771034	0.12009336406372	-0.01617520282291
N	-0.05846609206666	1.91206981115892	0.05781262634531
H	-0.13008160508690	-2.53202364230502	2.15803705622428
H	-0.13574417194687	-6.27814257131324	-0.00056621366601
C	-6.18121396826898	0.89185875352877	-0.05732304754248
C	-0.09282367806019	6.23483013056674	0.22354272494055
C	-6.52398663111751	1.75521548517368	-1.29711569657414
H	-6.26262587665493	1.23278717514391	-2.23084670364894
H	-5.99017008430527	2.71839211871372	-1.29138176573505
H	-7.60383481746910	1.97507346249947	-1.32107688721923
C	-6.56295635583676	1.66447245375376	1.23001977710063
H	-6.02994321020682	2.62481958163152	1.30993105522539
H	-6.33016254042300	1.07601909610390	2.13146954308472
H	-7.64320939665312	1.88358096961114	1.23629304994534
C	-7.01849306988093	-0.40071726874575	-0.11675094586238
H	-6.84108710773840	-1.04898612064609	0.75625612152141
H	-6.81303690686654	-0.98500144858320	-1.02794361948807
H	-8.09045549561761	-0.14867748248548	-0.12454692439427
C	-1.52943162452614	6.66479423469053	-1.03063675789924
H	-2.50421575325364	6.15647635530163	-1.09412818243794
H	-0.97354481844433	6.44050311812419	-1.95462853035798
H	-1.72250294103865	7.74965216035646	-1.00471654198858
H	-1.54676314047577	6.56423065562448	1.49685096796487
C	-1.00345894359360	6.26697261511327	2.40762875078055
H	-2.52198306290810	6.05288031638795	1.50640841866070
H	-1.74008869346372	7.64782830934104	1.55453563644176
C	0.58344308734705	7.04297633314028	0.26464980448522
H	1.20207158688560	6.87369458484992	-0.63111863179838
H	1.18945532730014	6.80345630035785	1.15296919951378
H	0.35461068120466	8.11938885873300	0.30544212987444
C	0.24693253513691	-2.32271807746427	-2.52509085654292
H	1.18475693172488	-1.74410274833806	-2.51369179633275
H	-0.56983977823738	-1.59668586546177	-2.67787111181921
H	0.26674457339750	-2.99977276381763	-3.39359561718724

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Aryl Chloride Triplet 2.4 Å Ni-C distance

Ni	-0.00033327531133	0.00039997778303	0.000153585432848
C	2.51298623249766	1.23475554280655	-0.28942092930195
C	2.73911109843192	-1.08089016748188	-0.11135022660404
C	3.90183324670844	1.37642055795075	-0.39716494189791
C	4.12491175732003	-0.99622445123151	-0.21373147368527
H	2.23195107237742	-2.04178100843601	0.00748877720270
C	4.75066208066023	0.25801347028665	-0.36462560806308
H	4.32508776147151	2.37764397191361	-0.50525822031622
H	4.70484962506387	-1.91902794342803	-0.17464635049458
C	1.53873061716178	2.33964854844818	-0.28871407751395
C	1.85309561295889	3.69991670740185	-0.39557353906163
C	0.84975521577871	4.68206654083057	-0.36188501418659
H	2.89939177101789	3.99454067557019	-0.50402670145422
C	-0.73026167128453	2.85374779554067	-0.10891039953792
C	-0.47285353075479	4.21810886319793	-0.21054246183176
H	-1.74702338054009	2.47080827184313	0.01024956226360
H	-1.31579952165603	4.90893613505728	-0.17057534976598
C	-0.00025403681827	0.00018076398129	2.40015357336634
C	-0.89586321861402	-0.78714161108814	3.14431360014892
C	0.93102223077594	0.81902702760450	3.03715235170505
C	-0.81994070547722	-0.72028286446491	4.55180529877515
C	0.99642996343343	0.87659264325664	4.44084654638347
C	0.11337972104715	0.10028073140735	5.19757745545184
H	-1.51017125650359	-1.32706007034276	5.15070585763721
H	1.73150668742226	1.52290483955783	4.93376093519236
Cl	-1.42137747155335	-1.25407191000864	-1.05499658488674
N	1.93426951067222	0.00016752105011	-0.15376760784819
N	0.24149186509379	1.91991800438949	-0.15259768147222
H	0.12367109484840	1.43205746545358	2.45176079219433
H	0.14808684070830	0.13086177846902	6.29140849463794
C	6.27328893097152	0.43012341451986	-0.48510239972805
C	1.21096902983854	6.17127703310790	-0.4817611886351
C	6.60414642385705	1.11021109422782	-1.83703085079084
H	6.25426470288997	0.50155109087432	-2.68569717179397
H	6.14046340434353	2.10514387879810	-1.92464515224266
H	7.69360788731015	1.24218971508391	-1.93949882206220
C	6.77934785267810	1.31932023698419	0.67810899204974
H	6.32367555969867	2.32164746545358	0.66184857379809
H	6.55318154309279	0.86423953163399	1.65517846320830
H	7.87145093369912	1.45080515030379	0.60830015233474
C	7.01508959534309	-0.91953997373502	-0.42434713637258
H	6.84459086895599	-1.44305625245078	0.52996193679322
H	6.71943262213670	-1.59195590378601	-1.24556446146617
H	8.09945570110735	-0.75070833895378	-0.51495721687240
C	1.92670321601323	6.41506980476315	-1.83377172650491
H	2.85579538964635	5.83058645913980	-1.92190119142047
H	1.27882326031925	6.14447766131448	-2.68238831358838
H	2.19391894419768	7.47950469662318	-1.93582458784312
C	2.15679216433792	6.56166961794242	0.68133946709460
H	1.67735056921534	6.39359773361188	1.65847609765649
H	3.09433604262082	5.98440162571119	0.66445801921644
H	4.2363916751397	7.62883218125500	0.61201458552797
C	-0.03527197236564	7.07606957672035	-0.42024009550982
H	-0.73966122886591	6.86725750948811	-1.24133416399927
H	-0.57570733609042	6.97199067968520	0.53418818028546
H	0.26786598377133	8.13083702414552	-0.51046295757589
C	-1.91739170637064	-1.68539627505681	2.48408695137284
H	-2.59649689269058	-1.11463978422370	1.83131861545725
H	-1.43808810846514	-2.43283187061550	1.83244112853718
H	-2.52709063864677	-2.22054085489056	3.22902533283277



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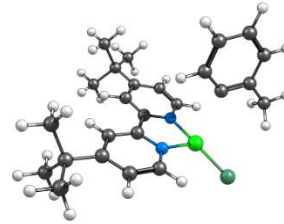
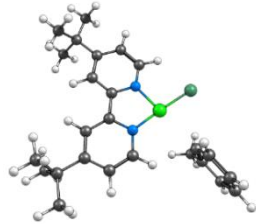
Aryl Chloride RKS 2.6 Å Ni–C distance

Ni	-0.00770113267897	0.05520537153822	-0.01332244578519
C	-2.37408388205711	1.44577168565359	0.01867323929238
C	-2.75152155587921	-0.85760293743260	-0.06284724153208
C	-3.74888112781657	1.68699357481028	0.01066752798148
C	-4.13047785617331	-0.66137251169919	-0.07341711681328
H	-2.31044268079458	-1.85440087771482	-0.08494175360262
C	-4.67861067914255	0.63364755906665	-0.03619900581071
H	-4.09799626414217	2.72166614075435	0.04014152322200
H	-4.76676204322600	-1.54673296767020	-0.11075389370268
C	-1.33578053518646	2.48232714724680	0.06396139127244
C	-1.55817692447162	3.86055427532408	0.12097972634267
C	-0.48405758274071	4.76769007016597	0.15984270729777
H	-2.58584298090329	4.23036528281285	0.13649583223060
C	0.97259085859237	2.81942968951109	0.08013889961759
C	0.80389003532536	4.20229195945503	0.13740523166729
H	1.95812660789498	2.34615677840156	0.06124627751129
H	1.69798967315434	4.82669472791733	0.16418628828236
C	-0.01350179958355	-2.54474636933309	0.00141873360247
C	0.12534281543865	-3.19652318582801	-1.22814364331755
C	-0.14838576636645	-3.23005376124726	1.20326135295173
C	0.09043589213079	-4.60673275858388	-1.21816728657769
C	-0.17692790294485	-4.63787939868382	1.19369832142954
C	-0.06059799463259	-5.32088391456953	-0.02166806832368
H	0.19407738132103	-5.15074951381670	-2.16488422345331
H	-0.28136335002364	-5.190111110601179	2.13394141829666
Cl	2.14104300786878	-0.15797667056645	-0.03446514919045
N	-1.85744875868983	0.16530457348772	-0.01733674957037
N	-0.06727829187728	1.96019316402783	0.04312008324825
H	-0.22282461810872	-2.68992912505833	2.15234786719487
H	-0.07803982237588	-6.41515492353291	-0.04072788991135
C	-6.18766350520227	0.91897052184738	-0.04496225739874
C	-0.74295057052942	6.28082887165169	0.22332607132301
C	-6.53765534575781	1.77875028828682	-1.28524394260893
H	-6.27711353362370	1.25567815118882	-2.21884088980161
H	-6.00768997733906	2.74406662231751	-1.28292632343880
H	-7.61843888061369	1.99423691956728	-1.30625469264435
C	-6.56858267329469	1.69227072236625	1.24221986222929
H	-6.03918483740374	6.265487309247626	1.31894930480655
H	-6.33077456138849	1.10626620057900	2.14395829171958
H	-7.64966441527536	1.90710301447855	1.25137980660119
C	-7.01990936671654	-0.37703959692990	0.09962642739690
H	-6.83726531912161	-1.02317129176171	0.77388376722213
H	-6.81501529323450	-0.96200129309947	-1.01050628998303
H	-8.09287722490138	-0.12926283297725	-0.10449078878676
C	-1.55144968640571	6.71244632016281	-1.02560539133149
H	-2.52563937202808	6.20249622898690	-1.08522924542389
H	-1.00001659847373	6.49139321013089	-1.95303885362221
H	-1.74633950563419	7.79688645435535	-0.99602675690213
H	-1.55526108016201	6.60608799332866	1.50167325122200
H	-1.00662150744918	6.30788236871713	2.40893466086837
H	-2.52957867862152	6.09311633070000	1.51539030565746
H	-1.75013028133336	7.68922559996473	1.56263507011024
C	0.56767600296570	7.09092107860792	0.25949330836034
H	1.18152632594028	6.92538495933251	-0.64025329981659
H	1.17898761436288	6.84958812910293	1.14368335807399
H	0.33741739418089	8.16684078614695	0.30483281745249
C	0.32616497193676	-2.42371772934538	-2.50987587062500
H	1.25219740539922	-1.82908188277525	-2.45500623600764
H	-0.449738622414490	-1.70934595880642	-2.67932060038218
H	0.38823675595829	-3.08727949902580	-3.38672751332689

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Aryl Chloride Triplet 2.6 Å Ni–C distance

Ni	-0.00021978645376	-0.00013033518081	0.00011320739657
C	2.51823574713735	-1.23638711028594	-0.12920595490962
C	2.73490987208914	-1.08343180623143	-0.00913317878795
C	3.90958579165888	1.37854600180062	-0.18319740895554
C	4.12389625585594	-0.99838685522527	-0.05572339426561
H	2.22291723685736	-2.04641287613001	0.06306159591772
C	4.75608888220771	0.25782761382240	-0.14979017111257
H	4.33725180131381	2.38163694637861	-0.24868133018702
H	4.70108275217847	-1.92301739323863	-0.01848225164109
C	1.54425181613395	2.34219248196074	-0.12807807340990
C	1.86096945422215	3.70450517605551	-0.18043590507986
C	0.85618870363724	4.68575764439253	-0.14479373472989
H	2.91001123904900	4.00210588904217	-0.24628022743098
C	-0.72947958118301	2.84995853138691	-0.00536976599915
C	-0.46972905373462	4.21712905248171	-0.05035035515398
H	-1.74936682973862	2.46364682380802	0.06721559548772
H	-1.31403772496335	4.90639431305856	-0.01150013547548
C	-0.00006969583450	0.00053349796149	2.60011311927436
C	-0.90118927285451	-0.78117714346536	3.33596191985533
C	0.93995388202431	0.81683943097047	3.21889106766440
C	-0.82037018353918	-0.71052423141149	4.74369795257889
C	1.00790156836028	0.87629664821230	4.62366644256914
C	0.12097178764858	0.10667911331203	5.38309809468972
H	-1.51253445468887	-1.31099685782230	5.34688051458450
H	1.74790646194919	1.51879845635186	5.11429429385382
Cl	-1.45876529497842	-1.28723611055073	-0.93297054964088
N	1.93235800434565	-0.00019168922588	-0.05097105308431
N	0.24366170120542	1.91704305944117	-0.04921898990084
H	1.63738368562077	1.42222818310176	2.62611027707778
H	0.15895334254857	0.14000558779376	6.47669235054713
C	6.28216722933276	0.43039536948624	-0.20954362638695
C	1.22006645230855	6.17792249763495	-0.20251701089325
C	6.66308561135284	1.14492817708275	-1.53017708556814
H	6.34479198394415	0.55884918401675	-2.40673277815957
H	6.203304516047491	2.14230457196743	-1.60904379115923
H	7.75562141596203	1.27831152107399	-1.58879845061222
C	6.74582493909238	1.28811479411453	0.99427192967742
H	6.29199461777912	2.29138977488826	0.98738665096826
H	6.48334358180106	0.80819697000753	1.95013489128328
H	7.83987754691698	1.41934731579603	0.96816042979478
C	7.02014928991728	-0.92167605423216	-0.15674158242606
H	6.81403988812187	-1.46956788125440	0.77662215019319
H	6.75443032075847	-1.57193821654063	-1.00557834553606
H	8.10727238100626	-0.75251918438360	-0.20283258866694
C	1.97587268013987	6.46767165292189	-1.52329235231452
H	2.90712706675184	5.88552391652884	-1.60385752904486
H	1.35357278400528	6.22735639216959	-2.39972891757133
H	2.24609898298580	7.53471206564650	-1.58041766454183
C	2.13045572947412	6.52770109995815	1.00110790680508
H	1.62209340170159	6.32631315731808	1.95708576744189
H	3.06842287000830	5.95094145542011	0.99247905486844
H	2.39867445304583	7.59648989786849	0.97649122298517
C	-0.02793907111889	7.08065838337821	-0.14720731894416
H	-0.70727659054978	6.90062653123694	-0.99577519736936
H	-0.59669271283064	6.94384755641031	0.78640365459917
H	0.27711149055904	8.13779317804370	-0.19179225040363
C	-1.92691102561183	-1.67154523478599	2.67227309901711
H	-2.59914800504043	-1.09366115358423	2.018730482066684
H	-1.44921033126913	-2.41967719502439	2.02034762018582
H	-2.54192510410158	-2.20389447330052	3.41475610797924



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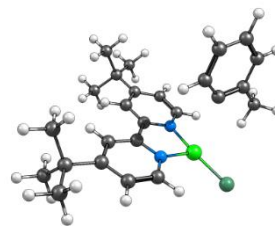
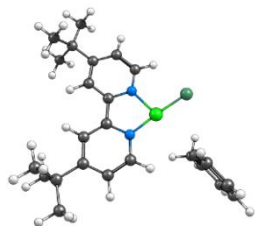
Aryl Chloride RKS 2.8 Å Ni-C distance

Ni	-0.00662734502564	0.11132445583695	-0.02164034320079
C	-2.37716470609225	1.48780067184539	0.01989688135138
C	-2.74367040469652	-0.81890972466228	-0.05908141405939
C	-3.75306999482194	1.72227657275186	0.01714062983605
C	-4.12366469022095	-0.62881277079481	-0.06387349526522
H	-2.29535883534303	-1.81256944241498	-0.08265529964038
C	-4.67741439267983	0.66379868171177	-0.02518308553332
H	-4.10756792339623	2.75512305426750	0.04705558375926
H	-4.75613564840590	-1.51701285679449	-0.09792293094947
C	-1.34187015104974	2.52792949511777	0.06052890848842
C	-1.56789458281861	3.90531788920580	0.11913665982728
C	-0.49651510610371	4.81602176887497	0.15276160353812
H	-2.96673029525863	4.27170454092560	0.13997160358852
C	0.96672945905118	2.87263178108812	0.06542079055782
C	0.79317424662068	4.25481243526661	0.12371835599513
H	1.95369905849542	2.40287271575307	0.04145924548312
H	1.68534161376475	4.88218023398611	0.14604021425896
C	-0.03196248019987	-2.68844330588573	0.00402279354473
C	0.16994855629585	-3.31284041278286	-1.22843116467314
C	-0.21556834708677	-3.38559643960807	1.18987224373156
C	0.14891555235054	-4.72396277651691	-1.24001280856243
C	-0.22948381810327	-4.79433395815434	1.15761291236340
C	-0.04954266683539	-5.45647397750543	-0.06144781447288
H	0.30072389471441	-5.25330287552085	-2.18866613373905
H	-0.37243725768299	-5.36198725763682	2.08361197696356
Cl	2.13906233665843	-0.11315685771548	-0.05562145140140
N	-1.85564670816258	0.20979933151539	-0.01748597789382
N	-0.07108218941207	2.01010807930963	0.03343876541079
H	-0.33989866528819	-2.85932264570560	2.14160304797533
H	-0.05475075027190	-6.55045240457381	-0.09723906932078
C	-6.18793520587527	0.94177532152420	-0.02790221652151
C	-0.76003092790165	6.32825771687603	0.21794957438480
C	-6.54721932003899	1.798542178660386	-1.26762285733339
H	-6.28803484458107	1.27574547340862	-2.20174925903286
H	-6.02199172472358	2.76645211015646	-1.26852424293796
H	-7.62911497187082	2.00870941311453	-1.28434074027432
C	-6.56722835258551	1.71455987994140	1.26007444121220
H	-6.04229767683552	2.67985441438936	1.33362452233451
H	-6.32282553305745	1.13067033805268	2.16142140204107
H	-7.64929776581123	1.92407794823403	1.27349956065109
C	-7.01411229862674	-0.35830037154137	-0.07776187541646
H	-6.82472427784123	-1.00264546934062	0.79563099859355
H	-6.81026285447130	-0.94321526340725	-0.98889943373674
H	-8.08826414524424	-0.11569264728286	-0.07836373540022
C	-1.57660965405824	6.75750300835187	-1.02654731574529
H	-2.54945269084186	6.24441083142110	-1.08110043179668
H	-1.02942630653516	6.53849502744119	-1.95697747482132
H	-1.77489295527400	7.84128511523708	-0.99564194680676
C	-1.56656537344786	6.65057921031726	1.50069445096260
H	-1.01208368374597	6.35408466552958	2.40495644981849
H	-2.53909076905768	6.13436586019694	1.51954295746884
H	-1.76474315781600	7.73304095674088	1.56287594825920
C	0.54811910514692	7.14262369158485	0.24726855181979
H	1.15773767692521	6.97918972977082	-0.65573667704407
H	1.16487556107943	6.90327452750745	1.12821209986721
H	0.31457839954887	8.21777355457894	0.29391554048715
C	0.41988484167948	-2.51509829414769	-2.48587578676405
H	1.33452741751129	-1.91050975193542	-2.37731728342880
H	-0.40413898191943	-1.80701083127365	-2.67735557361207
H	0.52887346527438	-3.16146958723449	-3.37090442518940

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Aryl Chloride Triplet 2.8 Å Ni-C distance

Ni	-0.23339825295833	0.31672933413110	0.02980916851563
C	2.34793557386758	1.38957362758977	-0.09583732301939
C	2.42424387060095	-0.93439012361820	0.06179349076132
C	3.74503372113968	1.45004798822525	-0.10245612400073
C	3.81596179813310	-0.93149091168077	0.05231954754645
H	1.85987884442203	-1.86707862359288	0.13718227341958
C	4.52506731188869	0.28341027110357	-0.03096719540341
H	4.23084025699005	2.42714453814728	-0.15574617419137
H	4.33550230506425	-1.88844322717410	0.11549319775323
C	1.44538690485343	2.55344175159496	-0.14935461660494
C	1.83908493205219	3.88800155500941	-0.29346756178928
C	0.89017525894823	4.92564028049674	-0.31116270873763
H	2.90168106092656	4.11991908605922	-0.39607458408230
C	-0.79780318563861	3.19580748263337	-0.05521655756640
C	-0.45916062491546	4.54165313324498	-0.18249277207213
H	-1.83637165085610	2.86610721394867	0.03206373428872
H	-1.26188803966610	5.28002092217764	-0.18349897280011
C	0.04760428065433	-0.07846333729126	2.78750028860161
C	-0.42382478066778	-1.26930111876788	3.34609644579490
C	0.63131896437956	0.93104609645760	3.53899297293963
C	-0.28599642143763	-1.41652809284375	4.74348638621671
C	0.76008487449486	0.76590208840265	4.93213122975155
C	0.29763604862006	-0.41238146159567	5.52795667634298
H	-0.64746228612970	-2.33549764904838	5.22149616479036
H	1.21368050893473	1.55587722075782	5.54131009839728
Cl	-2.18857756167897	-0.35858598522227	-0.56761921247504
N	1.68190292379901	0.19163034740721	-0.01452687583871
N	0.12392978849624	2.21226250013450	-0.03696196221555
H	0.98824210595053	1.85421198174102	3.06763142813237
H	0.38760786613582	-0.55262127128879	6.60984144105327
C	6.05941503629879	0.36687991339691	-0.0336683796526
C	1.32804834081130	6.38762214694195	-0.46775122223777
C	6.53239532143830	1.05824674348665	-1.33662796129554
H	6.21495297260998	0.49193895004074	-2.22645276714439
H	6.13474674655880	0.8079094994817	-1.43070478846275
H	7.63228589877557	1.12813115323845	-1.35258911516402
C	6.52558017251570	1.19581481172988	1.18932959354743
H	6.13025903045328	2.22336976873197	1.16756406285401
H	6.19878511590850	0.73160181718546	2.13297343000830
H	7.62563659709786	1.26390175082054	1.20559900306094
C	6.71447584495446	-1.02608445665272	0.04380079900886
H	6.44418888928144	-1.55964657129071	0.96902298037446
H	6.44034168701986	-1.66065678929927	-0.81428466750291
H	7.81065131919757	-0.92137416493127	0.03576722176743
C	2.08987596298790	6.54879785833289	-1.81263174065213
H	2.98577033649399	5.91079547174436	-1.86566759355670
H	1.44233348506970	6.28890355006062	-2.66481664646048
H	2.41847867504968	7.59297746040705	-1.94124719282084
C	2.28472851375597	6.75901624697380	0.70086397823886
H	1.77892533367128	6.65112393433120	1.67327134093915
H	3.18666199160863	6.12766194706388	0.72023653107678
H	2.61532775291211	7.80595098561244	0.60386069564891
C	0.14506385233706	7.36337187440315	1.67327134093915
H	-0.55455338240889	7.17171820597873	-1.28592680151705
H	-0.41863322663411	7.31750967075040	0.48883600170297
H	0.5101129297228	8.39612410596760	-0.56956735111391
C	-1.05033661993656	-2.35884311282704	2.50515181775003
H	-1.85016324184354	-1.95960534446841	1.86315586867779
H	-0.38042314750713	-2.8182897234936	1.82854855475449
H	-1.47045543285360	-3.16347238946739	3.12874259017545



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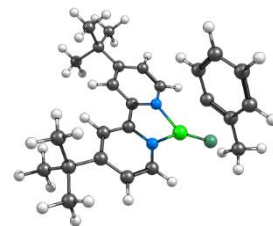
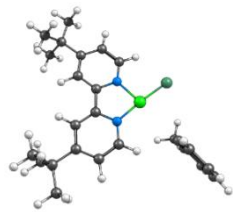
Aryl Chloride RKS 3.0 Å Ni–C distance

Ni	-0.00053890017017	-0.00035490097041	0.00237186298748
C	-2.40522862362958	1.31198629538896	0.02280342063902
C	-2.71026434576332	-1.00270530322071	-0.10464061394748
C	-3.78639495496829	1.51121712871430	-0.00132483471142
C	-4.09440422651761	-0.84746865395024	-0.13172140400797
H	-2.23372761578673	-1.98311193725512	-0.13766012829969
C	-4.68172104218000	0.42986139889393	-0.07961755174112
H	-4.16838305358899	2.53381332120895	0.04039545058057
H	-4.70322192617393	-1.75052151554081	-0.19389994457738
C	-1.39661029567407	2.37646944360363	0.10003973432094
C	-1.65690777487789	3.74675160944162	0.17872280352854
C	-0.60900147029658	4.68274124428418	0.24556764565992
H	-2.69475133779749	4.08737161076728	0.18914629131831
C	0.90346219498387	2.77735526180657	0.14918094666719
C	0.69448458423809	4.15360011364232	0.22810823307923
H	1.90209717297316	2.33294093122101	0.13371471771587
H	1.57046530149370	4.80204684077325	0.27562908875712
C	-0.00082103157137	-3.00035319511116	-0.00081609105138
C	0.31299130344723	-3.57801282400207	-1.23079459712940
C	-0.26240714201741	-3.7302252847092	1.14800944234412
C	0.32691025277117	-4.98887954215049	-1.28219032509111
C	-0.24011442095790	-5.13824815107652	1.07543954124860
C	0.05276324661763	-5.75917614020731	-0.14332727354466
H	0.56576832135518	-5.48743157102742	-2.22972744089504
H	-0.44375135007132	-5.73628124206229	1.97058085102263
Cl	2.14639426363309	-0.19191946529427	0.00378859330478
N	-1.85107895429131	0.04854650628006	-0.02707868157313
N	-0.11259433403914	1.89046933311961	0.08512549916017
H	-0.47477403464797	-3.23471856573486	2.10098456831561
H	0.07670057447400	-6.85148365603410	-0.20955869649859
C	-6.19870598706274	0.66896323499938	-0.10469846675324
C	-0.91065283396444	6.18669412238427	0.33223852743265
C	-6.55832504425926	1.53835843115253	-1.33549021977534
H	-6.26926189577064	1.03931755931477	-2.27382688091559
H	-6.05864428124712	2.51937482175740	-1.30995171862974
H	-7.64486484575427	1.72084441790127	-1.36799924564888
C	-6.62033704307250	1.40856521947864	1.18962703615537
H	-6.12240344655664	2.38573521150527	1.28914811884310
H	-6.37622808812443	0.81531067854835	2.08491304962950
H	-7.70760945341490	1.58957744050553	1.18752646645450
C	-6.98988589886349	-0.65073574833100	-0.19201749721242
H	-6.79919989049215	-1.30552758968895	0.67328085413772
H	-6.75517639802079	-1.21393660027753	-1.10938692338166
H	-8.06977780540152	-0.43570170297157	-0.20761586648569
C	-1.71771035346242	6.61763798514689	-0.91787916761914
H	-2.67656979922485	6.08193047822700	-0.99713395094729
H	-1.15053891304122	6.42855887971502	-1.84288625402795
H	-1.94326687137880	7.69551239609460	-0.87154882211976
C	-1.74518593784334	6.46682796124111	1.60699609489976
H	-1.19818974212810	6.16783931135497	2.51498313855186
H	-2.70504557797452	5.92717268519246	1.60093408015451
H	-1.97061573720272	7.54293498506086	1.68459222542197
C	0.37642111595759	7.03199848796451	0.39684358615043
H	1.00420287734715	6.89934171467312	-0.49874447035370
H	0.98476425541530	6.79242290338457	1.28355665974771
H	0.11572524634562	8.10014499513538	0.45803975737642
C	0.64069896010306	-2.73582536862322	-2.44067734021337
H	1.52578156606985	-2.11097716567511	-2.24121720854679
H	-0.18530087674957	-2.04332470963478	-2.675306337969738
H	0.83684905780583	-3.35164145157270	-3.33240983420929

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Aryl Chloride Triplet 3.0 Å Ni–C distance

Ni	-0.30654256249307	0.32426947963475	-0.11818174730212
C	2.28667169066254	1.36524398706220	-0.13404719117021
C	2.32940525954338	-0.96125167165738	-0.01057726826229
C	3.68333163912174	1.40723950257852	-0.11745601628568
C	3.72145016959098	-0.97621862354421	0.00758056071847
H	1.75277842377944	-1.88843051201726	0.03535060739238
C	4.44766859694098	0.22945510435530	-0.04516181526184
H	4.18273763847227	2.37816273594398	-0.15635293077841
H	4.22698670013327	-1.94101235695309	0.06591376055834
C	1.40016974251561	2.54104462627337	-0.19755577169338
C	1.81343128893477	3.87347373598046	-0.29185412987574
C	0.87689581920707	4.92222141219178	-0.33366494523330
H	2.88214023304717	4.09610417338970	-0.33398185457278
C	-0.83796451094528	3.20530400201571	-0.19761176279466
C	-0.48052882783387	4.54993667244389	-0.28043520582903
H	-1.88305439991227	2.88603453710729	-0.16623926065746
H	-1.27522293591495	5.29660534623470	-0.30573587103980
C	0.03062905889372	0.09715109722025	2.85414604964437
C	-0.17221416120251	-1.19067440283602	3.34361438672952
C	1.81343128893477	1.18051919492321	3.64928871627441
C	-0.00316873807393	-1.37254943837142	4.73551096326342
C	0.53704476873734	0.97813455131130	5.03254889755344
C	0.34678777226167	-0.30297742621667	5.56794750855571
H	-0.15421385924252	-2.36978792832579	5.16790099736049
H	0.80626136061880	1.81693840834198	5.68416758457215
Cl	-2.23314334616231	-0.43187442822788	-0.68302338996356
N	1.60205385149242	0.17568616714522	-0.07703735511230
N	0.07164096349418	2.21067255291052	-0.15510974210886
H	0.51763403214027	2.17939696375645	3.22200597273730
H	0.46859349141769	-0.46960533169278	6.64287501884717
C	5.98260165122551	0.29338671839914	-0.01948966357185
C	1.34659090027479	6.38215584904634	-0.43815589973128
C	6.48793472667830	0.99078197533108	-1.30702779350207
H	6.17960009419101	0.43688861351883	-2.20780567032666
H	6.10495712128162	1.01914805541973	-1.39854154168016
H	7.58874831648346	1.04683525326138	-1.30245960294471
C	6.43702359106152	1.10484482205348	1.21954295175447
H	6.05464510116076	2.13733398951406	3.22200597273730
H	6.08758610177931	0.63598879420134	2.15271015707740
H	7.53737783257526	1.15918694407050	1.25602789965948
C	6.1844079837124	-1.10851527275036	0.05645858834276
H	6.32312727875255	-1.64765257544732	0.97075424590454
H	6.35318287187299	-1.73096911223454	-0.81322150215992
H	7.71581459027202	-1.01786091033249	0.07087318132021
C	2.16640572259805	6.56422990910514	-1.73697216646469
H	3.05722690057101	5.91737024438539	-1.75941495233338
H	1.55973371943193	6.33023068672290	-2.62595975206280
H	2.51176796551693	7.60715905086566	-1.82580917224210
C	2.23735998455309	6.71797800932568	0.78693188800558
H	1.68224452309630	6.59575128908355	1.73031663112420
H	3.13030873518515	6.07574301129912	0.83795460175889
H	2.58361664475997	7.76277203424872	0.72910299681520
C	0.16426908518183	7.37048092442306	-0.46194655569608
H	-0.49485328006768	7.20444231280352	-1.32904866155710
H	-0.44648386394491	7.31019479139683	0.45305765480116
H	0.54455404085180	8.40143474258741	-0.53352848276019
C	-0.55909354715347	-2.34305968858741	2.44307201259200
H	-0.64025583066622	-1.99735891785407	1.40262632896746
H	0.17647352515094	-3.16475219008685	2.48969382072122
H	-1.53913243103860	-2.76545915210825	2.71954554625357



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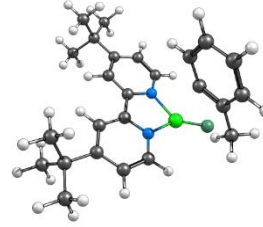
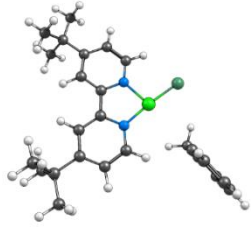
Aryl Chloride RKS 3.2 Å Ni–C distance

Ni	-0.02966723908317	-0.06228859722122	-0.02929559348089
C	-2.48565865207225	1.14725769034812	0.00810447418419
C	-2.69452832086321	-1.17792342760763	-0.14126795509181
C	-3.87387033521965	1.28926593965068	-0.01226800381691
C	-4.08397889030588	-1.07954674365756	-0.16402878810646
H	-2.17564411395884	-2.13651128745845	-0.18483351182174
C	-4.72336746064478	0.17195754035860	-0.09866690496643
H	-4.29824198591277	2.29461679161069	0.03867994925721
H	-4.65512640599281	-2.00632700524857	-0.23379136545683
C	-1.52035540289928	2.25093187934497	0.09280608156559
C	-1.83443719970694	3.60869318832633	0.18796023228499
C	-0.82437926952524	4.58515349857608	0.25937427106214
H	-2.88502646419738	3.90731271125024	0.20818106274333
C	0.76319554738997	2.74345114902550	0.13541059245239
C	0.49928051752826	4.10919251787949	0.22944347177059
H	1.77879842299587	2.34021428062592	0.11116772938142
H	1.34865508014563	4.79196495289949	0.27918263832770
C	0.02831951057755	-3.26176290734091	-0.02796442534279
C	0.40940094590461	-3.78825317354695	-1.26068636776737
C	-0.26103002681338	-4.02949120760986	-1.08743309507535
C	0.46661891166919	-5.19637786719951	-1.35296976044041
C	-0.19521531579132	-5.43411078377188	0.97347712177524
C	0.16696084638193	-6.00804854840715	-0.24966139981324
H	0.75914061106677	-5.65927512711533	-2.30367951572965
H	-0.42032658372590	-6.06531450462343	1.84040041155008
Cl	2.11827875986026	-0.19175076191128	-0.03438625785606
N	-1.88045005406950	-0.09162812523153	-0.05455535830305
N	-0.21750727398503	1.81752327840768	0.06695802357247
H	-0.52809852912914	-3.57029028110495	2.04524581168437
H	0.22508541391758	-7.09673648617337	-0.34714873629900
C	-6.24908813332774	0.34797521661191	-0.11906388827290
C	-1.18553538350415	6.07477979176419	0.36410648543590
C	-6.64686032559229	1.21249139434573	-1.34152960310886
H	-6.33925030108239	0.73411784271942	-2.28471720097152
H	-6.18823548038468	2.21313907478716	-1.30813166563374
H	-7.74008924511838	1.35003577988728	-1.37064213326062
C	-6.69858479720175	1.05793339456037	1.18245232015978
H	-6.24207440555913	2.05432057700067	1.289678307782030
H	-6.42788528299548	0.46772410787587	2.07208510417745
H	-7.79250159696247	1.19302559847660	1.18381254368590
C	-6.98486978423861	-1.00268038330196	-0.21674534103716
H	-6.76492502357837	-1.65669713052674	0.64216202458760
H	-6.72930109124780	-1.54741833120304	-1.13966315166892
H	-8.07280085555641	-0.83263299648707	-0.22811902880012
C	-2.01634581971680	6.48645100949049	-0.87692175866761
H	-2.95336452325906	5.91353237298233	-0.95716499624872
H	-1.44729917616728	6.33050671608082	-1.80694455954012
H	-2.28475399860464	7.55379867849368	-0.81740199484094
C	-2.02325750907487	6.30744401272625	1.64630437213123
H	-1.45960620769717	6.02066625135823	2.54801730787402
H	-2.96089031409759	5.73005881289250	1.63932851495273
H	-2.29094950006443	7.37277568696685	1.73702686560357
C	0.06700131381961	6.97031281718461	0.43112809832021
H	0.69448310911501	6.87252623050323	-0.46914550156953
H	0.68945859240392	6.74598419764067	1.31201613122709
H	-0.23592602369177	8.02641785007359	0.50527469506739
C	0.76085661207037	-2.89783595681143	-2.42893050369406
H	1.62258365847055	-2.25948894686277	-2.17706247176900
H	-0.07257890313193	-2.21591063595442	-2.66779752846414
H	1.00238950943481	-3.47787557934932	-3.33342366088961

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Aryl Chloride Triplet 3.2 Å Ni–C distance

Ni	-0.00005425733343	0.00014639961367	0.00003391203456
C	2.51124187063200	1.22593722527406	0.10896718256125
C	2.71328450437449	-1.07077027010542	-0.25690651268584
C	3.90010330456494	1.37461233815992	0.05412221535019
C	4.10303584578800	-0.97984535343981	-0.31362852935321
H	2.19093021632313	-2.02306230825949	-0.38161862406695
C	4.74057737445095	0.26641019727967	-0.15822676729223
H	4.33285473465289	2.36989317673712	0.17959077972989
H	4.67546232468588	-1.89295968338359	-0.48192775196823
C	1.53453499452331	2.30762052120006	0.32808261939946
C	1.85064939283218	3.65368823984073	0.52629853379699
C	0.84674602604160	4.61723127653900	0.73008474486521
H	2.90090335002662	3.95481963063227	0.52407012936891
C	-0.73852717699246	2.78791423466882	0.51211597974179
C	-0.47842062689809	4.14053619566074	0.71514585860881
H	-1.76155325045451	2.40359340695257	0.50176196293553
H	-1.32482817904116	4.81263587128760	0.86274765197702
C	0.00010135343780	0.00000197746832	3.20003390373280
C	-1.31433284941974	0.03779437526068	3.65259131879683
C	-0.39049799728877	-0.00249521422326	4.02151548020559
C	-1.48980519414666	0.08522311379907	5.05500634736818
C	0.91516396176272	0.04391782872956	5.41441597089857
C	-0.39049799728877	0.08858006329859	5.92198974432542
H	-2.50640442263968	0.11557622838803	5.46679805343663
H	1.77455310960702	0.04205877207888	6.09397513531893
Cl	-1.16225736968858	-1.65850455117383	-0.69690215074242
N	1.92019555007335	0.00014800669005	-0.04909767111610
N	0.23270645519628	1.86579922442754	0.32588866953133
H	2.13066227881084	-0.04158284786602	3.61207668141166
H	-0.55406254822016	0.12313956340008	7.00361114507540
C	6.26610947621015	0.44520907344228	-0.21349446433827
C	1.21248483377730	6.09223126907839	0.95614596755111
C	6.62485056789746	1.41225395488430	-1.36934379443281
H	6.28463614660838	1.01706482721432	-2.33950454126054
H	6.17021335012357	2.40601111940014	-1.23428164899777
H	7.71687043242882	1.55195256190890	-1.42307807205858
C	6.75923946752600	1.04039669077344	1.12902300909438
H	6.30795625987289	2.02296998813491	1.33730951782996
H	6.51728086700749	0.37491184157561	1.97262663718014
H	7.85282703109415	1.17615436440093	1.10586524018003
C	6.99744067575181	-0.89039185632573	-0.45170131478998
H	6.80560345640667	-1.61688461171685	0.35408634685616
H	6.71204615358196	-1.35358444748502	-1.40976352478962
H	8.08449179287115	-0.71730548104867	-0.48355757118451
C	1.99036371941745	6.62145506345287	-0.27449400206859
H	2.92205693018622	6.06063477467824	-0.44777407544249
H	1.38231465859708	6.55217859930613	-1.19032752824313
H	2.26318314290944	7.67914750969811	-0.12653220889647
C	2.10294886225384	6.20821330104968	2.21857356602592
H	1.57838957610029	5.83393862791580	3.11160780908170
H	3.03965537391469	5.63809542846765	2.11785708793579
H	2.37352935837938	7.26163969075307	2.39794457782866
C	-0.03604340512877	6.97290961148726	1.15855770290728
H	-0.70119652277142	6.95629208034579	0.28023671409624
H	-0.62017392808342	6.66552034344488	2.04069533153758
H	0.26943382169612	8.01895158439566	1.31722509775604
C	-2.49294577945819	0.01874228463116	2.70536638134371
H	-3.16695198192637	0.87662249890543	2.86991704337478
H	-2.13561107907426	0.03808510445606	1.6566285611816
H	-3.09276903958773	-0.89897777287036	2.81979104355909



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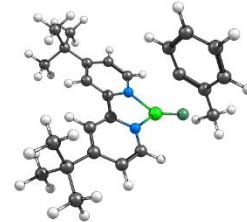
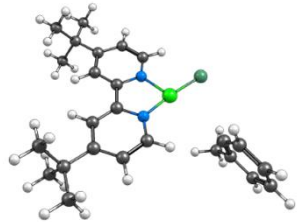
Aryl Chloride RKS 3.4 Å Ni–C distance

Ni	-0.00017893471236	-0.00024475468956	0.00184845822685
C	-2.46768238949029	1.18487287376308	0.02382010827172
C	-2.65362848133260	-1.14447987830255	-0.10259793602616
C	-3.85708329067306	1.31336093490541	0.00120687385777
C	-4.04395359659154	-1.05942332426018	-0.12736565427421
H	-2.12414169004662	-2.09813623140883	-0.13561777105958
C	-4.69527957969178	0.18663714149686	-0.07556696659771
H	-4.29154718516877	2.31482063513266	0.04333218184275
H	-4.60621204976288	-1.99225481273665	-0.1875908805867
C	-1.51178438113796	2.29756592468407	0.10296200217332
C	-1.83644060177921	3.65372585440080	0.18249456328996
C	-0.83427143508826	4.63839791703680	0.25340156443789
H	-2.88939528084649	3.94456631202044	0.19025535286218
C	0.76858528148268	2.80820174756257	0.15939349339368
C	0.49330550084797	4.17253661362427	0.23940678190161
H	1.78753702047606	2.41340380968675	0.14623265448510
H	1.33689622112073	4.86235524360892	0.29033777627737
C	-0.00006143329882	-3.40024421833917	-0.00006151783200
C	0.40674460627790	-3.86820090930321	-1.24748442830839
C	-0.32681874685589	-4.21530788804334	1.06931269398022
C	0.45276300556166	-5.27100734707226	-1.40703048353080
C	-0.27229686747656	-5.61395810146134	0.88795574562149
C	0.11612245498086	-6.13144116961559	-0.35217611547649
H	0.76539056226425	-5.69099407830659	-2.37127927574585
H	-0.52744915579569	-6.28436597657168	1.71642731852157
Cl	2.14357998093372	-0.14002450607777	0.00236911527190
N	-1.85093738601399	-0.04847970734164	-0.02769487474552
N	-0.20511757395055	1.87459832066649	0.09139375422250
H	-0.61465466803486	-3.80166929752528	2.04228664172232
H	0.16589982394616	-7.21472662520168	-0.50101251518929
C	-6.22264606360656	0.34739090155999	-0.09930025663763
C	-1.20753120891140	6.12616364261164	0.34062995433713
C	-6.62734941883466	1.19757876961902	-1.32952478762291
H	-6.31369330114667	0.71439012450617	-2.26825113862445
H	-6.178914877115429	2.20307564408617	-1.30397256284278
H	-7.72185414172585	1.32386094996293	-1.36117553393154
C	-6.68070180434105	1.06387171310933	1.19563849579081
H	-6.23384674738268	2.0654322326748	1.29515906887624
H	-6.40568465563897	0.48368308147348	2.09052046546740
H	-7.77584951205249	1.18853823275905	1.19439562099017
C	-6.94493876244450	-1.01123857773635	-0.18652820798264
H	-6.72038331265671	-1.65558891101490	0.67845608124846
H	-6.68215414171469	-1.56144278025828	-1.10415049522854
H	-8.03445023034234	-0.85195812663520	-0.20144742169778
C	-2.03000208826021	6.51959831222599	-0.91184703732476
H	-2.96194336636383	5.93888046445119	-0.99506129991410
H	-1.45130850007351	6.35905964312357	-1.83510558439659
H	-2.30687989065832	7.58540218577545	-0.86506536498180
C	-2.05866251322676	6.36464708554112	1.61288179221477
H	-1.50108312644308	6.09096839791254	2.52240774625939
H	-2.99178804500510	5.78004890606887	1.60305117913588
H	-2.33527783246375	7.42869674508986	1.69082109610184
C	0.03756767443613	7.03178935399035	0.41040142176399
H	0.67382820337529	6.93049915374148	-0.48330315090389
H	0.65378214361593	6.82058691291768	1.29889901616076
H	-0.27400725149862	8.08618067281464	0.47189119372878
C	0.79468929003166	-2.92387533139729	-2.36114303860808
H	1.65024808576644	-2.30134732926435	-2.05483923019328
H	-0.03001348426271	-2.22755470525807	-2.58887328484277
H	1.05958330583951	-3.46004582037538	-3.28592638485755

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Aryl Chloride Triplet 3.4 Å Ni–C distance

Ni	-0.00161283009671	0.00025304921980	0.00053141904558
C	2.50344283571986	1.21866697197054	0.23283101473594
C	2.71685666457783	-1.06592491282778	-0.19724837715637
C	3.89347261097800	1.36349884076922	0.24943383873479
C	4.10795613763922	-0.97814475064710	-0.18777360363351
H	2.19860601774561	-2.01197688427486	-0.37562028664708
C	4.74054758266294	0.25959132009392	0.03967879857634
H	4.32203147693278	2.35211896814621	0.43033990562977
H	4.68553833877428	-1.88718603988601	-0.36064371581610
C	1.51871012965708	2.29642694059733	0.43263311949357
C	1.82429616751005	3.64046231385493	0.65704786400484
C	0.81160949153777	4.60136457476008	0.82916401787602
H	2.87352002581641	3.94268820775987	0.69790495585345
C	1.067136208851018	2.77293104917971	0.52717521957368
C	-0.51128038892267	4.12358437851287	0.75362753030722
H	-1.78251538216714	2.38764472506864	0.46950138920536
H	-1.36389264356038	4.79381147520775	0.87132792562629
C	0.00411121394320	-0.00313365107224	3.40052491603511
C	-1.33778159500931	0.05315909233220	3.75548569511074
C	1.06573633764862	-0.00511728290399	4.28768980775304
C	-1.60406002782482	0.12226842994923	5.14303513031831
C	0.77221306358332	0.06294713399495	5.66339302107386
C	-0.56426929136518	0.12735172078716	6.08073550633684
H	-2.64527382408491	0.16878690168370	5.48562672538058
H	1.58397160959830	0.06300590546029	6.39894854844395
Cl	-1.15999524583745	-1.66784428649163	-0.67339945150062
N	1.91695160612997	0.00056536713104	0.00839678750901
N	0.21797615799245	1.85209860230874	0.37403998842016
H	2.10464172040359	-0.05950497013217	3.94515416964547
H	-0.79930089954968	0.17928762842508	7.14830566978812
C	6.26742646609057	0.43403646881103	0.06281110499417
C	1.16578324779211	6.07432967887296	1.08475742680308
C	6.68302050040579	1.43885580860036	-1.04059496622766
H	6.38769541465674	1.07896989631927	-2.03879841442571
H	6.22514675613522	2.42926979837057	-0.89250525921899
H	7.77675091702716	1.57565141415810	-1.03814338116143
C	6.69803812050744	0.98069394331579	1.44680489281817
H	6.23849677627728	1.95657861284827	1.66803245947840
H	6.41609344735244	0.28680437265063	2.25435112148905
H	7.79168901870394	1.11415942769120	1.47956532294879
C	7.00605831917283	-0.89548082124186	-0.18660610954178
H	6.77427557471247	-1.64855394000580	0.58348675946120
H	6.76523303942623	-1.32414992724266	-1.17257846042517
H	8.09384776223273	-0.72592229902396	-0.16091257388687
C	1.99675419416083	6.61603210644994	-0.10507897199763
H	2.93619987334634	6.05807552233225	-0.24189100170834
H	1.43014309980256	6.55442747495942	-1.04764250366372
H	2.26102744954690	7.67266001880897	0.06457918889615
C	1.99953707015614	6.17882038934526	2.38627931619225
H	4.3611750398298	5.79639823844475	3.25178416225948
H	2.93974969260469	5.60922200062229	2.32168266077284
H	2.26182840303148	7.23049248009065	2.58721230264583
C	-0.09128454569994	6.95245352545441	1.23998481823834
H	-0.71719519572905	6.94292702993689	0.33317260498317
H	-0.71332462846095	6.63700291967064	2.09288898742557
H	0.20581682956930	7.99728923042556	1.42104983615452
C	-2.44787011453185	0.02876766185253	2.72963026720054
H	-3.14650089068659	0.87216828039370	2.86041858776194
H	-2.02118279752340	0.06935175345413	1.71683520121639
H	-3.03600200398527	-0.90151151978284	2.78938311879302



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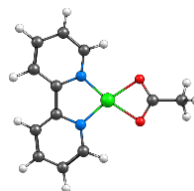
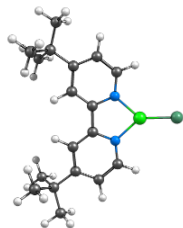
Aryl Chloride RKS 3.6 Å Ni-C distance

Ni	-0.00007248830926	-0.000181422256916	0.00123139967598
C	-2.50491137499401	1.10516674783016	0.01598504580161
C	-2.61422754968785	-1.23180571251961	-0.07612830171734
C	-3.89774101770213	1.18766810847804	-0.00544023671944
C	-4.00667448602127	-1.19248392258418	-0.09787146776416
H	-2.05204349543135	-2.16753285098600	-0.09400751147371
C	-4.69810405495508	0.03248277129606	-0.06443184598825
H	-4.36522076389975	2.17463084773266	0.02445002612474
H	-4.53835913655155	-2.14396234959101	-0.14100643893963
C	-1.58390889766433	2.24802395604488	0.08337256082652
C	-1.94906859656037	3.59463263837104	0.14599553769761
C	-0.97687785633307	4.60944391674036	0.21110502885323
H	-3.01029806256481	3.85387554402689	0.14509121347727
C	0.68081468784873	2.82752853958138	0.14483758193411
C	0.36423735028732	4.18364063302298	0.20914623128723
H	1.71134146050100	2.46418752455369	0.14033424231788
H	1.18637867076020	4.89907977658406	0.25721946060754
C	-0.00018837291810	-3.600181115340533	-0.00013098762629
C	0.38460130794399	-3.96310984283097	-1.28866376496688
C	-0.29948953603010	-4.49894169675816	1.00781714275392
C	0.44084865707157	-5.34880395861704	-1.55967104997101
C	-0.23599261629048	-5.87864907441252	0.71492956316276
C	0.13302416593943	-6.29263751176158	-0.56927575564974
H	0.738377991011170	-5.68868383497913	-2.55968468532085
H	-0.47045502068571	-6.61498280386157	1.49209257151858
Cl	2.141144904610402	-0.10655673314841	0.00182002557239
N	-1.84877854015043	-0.10784081767337	-0.02264821720568
N	-0.26480910698975	1.86513180149241	0.08252787910680
H	-0.57348979953190	-4.16791432092802	2.01624075115259
H	0.18980869174824	-7.36030741043176	-0.80382359361554
C	-6.23001262019064	0.14250098108680	-0.08826072306674
C	-1.39479361020958	6.08623364753011	0.28030272986509
C	-6.66360739581947	0.95927165965115	-1.33122097406269
H	-6.33522348553041	0.47169573016635	-2.26261133031127
H	-6.24838678113363	1.97922991551285	-1.3223525845185
H	-7.76169415790665	1.04902065042180	-1.36321109591024
C	-6.71031028882989	0.86384028597147	1.19586789591410
H	-6.29700727662080	1.88119337802514	1.27889239486027
H	-6.41533921290921	0.30734981275009	2.09940073539613
H	-7.80898767401609	0.95198110584802	1.19425410809932
C	-6.90714495410126	-1.24043716002419	-0.15300292744193
H	-6.66080754175492	-1.86321926254997	0.72178512375092
H	-6.62706638511990	-1.79621748251328	-1.06209424418163
H	-8.00132540231187	-1.11742508788436	-0.16903086937409
C	-2.22305440159664	6.44119852399281	-0.97983533794591
H	-3.13687216659759	5.83204803518881	-1.06055294135377
H	-1.63571854839061	6.28813052220833	-1.89889087891993
H	-2.53185693175977	7.49866772385850	-0.94582052157209
C	-2.25839217746163	6.31281032623617	1.54633434080302
H	-1.69699722997261	6.06582802628266	2.46113877334038
H	-3.17358057743772	5.70047354009552	1.53896724311000
H	-2.56701857439556	7.36887435333971	1.61144114125930
C	-0.17766764310001	7.02946095218625	0.34526987391236
H	0.46552134750588	6.93733280805569	-0.54445843335295
H	0.44038947664709	6.84688455456976	1.23882634250511
H	-0.52094867046421	8.07464275259868	0.39345698720368
C	0.73941597336894	-2.92894665323644	-2.33186529143704
H	1.09785659506803	-2.32463211689856	-1.99837181306035
H	-0.09546862465836	-2.22329782905784	-2.48134585904749
H	0.98414805875431	-3.38553351710880	-3.30374159344191

60

Aryl Chloride Triplet 3.6 Å Ni-C distance

Ni	0.00001768673953	-0.00001575769997	0.00006430360850
C	2.50388778285659	1.20667502804049	0.28752835596190
C	2.71716262083744	-1.06138389069967	-0.22372704700920
C	3.89370736928023	1.34449482563069	0.33746014870825
C	4.10814095879256	-0.97952367720141	-0.18618426004869
H	2.19876293860601	-1.99806161257817	-0.44613210675998
C	4.74072760272042	0.24575611790912	0.10138669121438
H	4.32200880118163	2.32315243169668	0.56700410642787
H	4.68581665187883	-1.88347425513342	-0.38382822581644
C	1.51835907350625	2.28005488956824	0.50371986112884
C	1.82080816554007	3.61935900233630	0.75166723952099
C	0.80598723206309	4.57651725795081	0.93883235906060
H	2.86956217822779	3.92130855280873	0.81234818848077
C	-0.76355661937018	2.75410412743964	0.58448886179169
C	-0.51605897897983	4.09988582537202	0.83957218508044
H	-1.78371800408436	2.36925147493148	0.50862182020257
H	-1.37008711332649	4.76758861427485	0.96158316605345
C	-0.00007937105396	0.00026316956645	3.60006428442219
C	-1.36147080642628	0.05630399012894	3.86485101000083
C	1.00931323929683	0.02579952124489	4.54418071389347
C	-1.70973771169216	0.15731628285259	5.23259144156188
C	0.63168127822319	0.12490955906530	5.89754715816597
C	-0.72819240983118	0.19110928554294	6.23062396580948
H	-2.76987172249311	0.20629194499051	5.51026517000617
H	1.39722908768625	0.14811063711419	6.68051851350028
Cl	-1.16158346072015	-1.67673540532504	-0.64289279826538
N	1.91689358046771	-0.00001624143615	0.00675846047789
N	0.21784837277303	1.83565957164096	0.42380238353292
H	0.06648503298911	-0.02994487169338	4.26410072715083
H	-1.02786455215465	0.26767173025109	7.28028695263460
C	6.26744839522669	0.41225350013574	0.16218662372092
C	1.15685218510453	6.04454503602685	1.22541222576264
C	6.70947322485315	1.45968303297919	-0.89009720934562
H	6.43351838053356	1.14237903995420	-1.90810075948306
H	6.25219257680102	2.44519389207082	-0.71082816530127
H	7.80341591696244	1.59147924399149	-0.85965841759588
C	6.67180113046612	0.89950377608190	1.57600857929103
H	6.21136493679982	1.86753569069703	1.82782595259829
H	6.37061968162486	0.17421884395503	2.34826249839823
H	7.76507021732652	1.02646133456757	1.63660817750000
C	7.00614803566049	-0.90918139703982	-0.12684743998565
H	6.75669504733337	-1.69194410770971	0.60727404231546
H	6.78298638786741	-1.29639489129400	-1.13391532815234
H	8.09384013059190	-0.74552281789167	-0.0718687304589
C	1.99056936890403	6.61120533792600	0.04915121678901
H	2.93059803035840	6.05645730975744	-0.09653238269810
H	1.42645784857832	6.56826683477514	-0.89594708788360
H	2.25368563866933	7.66439439454138	0.24087526168304
C	1.98640793481074	6.12520849805580	2.53127767761837
H	1.42129174612040	5.72431553839257	3.38728104460468
H	2.92829538255196	5.55940246752029	2.45826665978887
H	2.24564029611414	7.17328554936989	2.75387255890565
C	-0.10222549426171	6.91725872428035	1.39433499180456
H	-0.72404259834646	6.92717674635027	0.48472371047745
H	-0.72760297922039	6.58163305170114	2.23706089475412
H	0.19236330789369	7.95827288450305	1.59996722131141
C	-2.40660955258228	-0.00191594365600	2.77467386229897
H	-3.14164105083609	0.81462152237274	2.86858748281095
H	-1.92619739358251	-0.05834147226499	1.78705557369468
H	-2.96244534585768	-0.95343024110644	2.79722317386600



46

Aryl Chloride Putative Ni(I) Doublet—Phenyl Dissociated

Ni	1.12131625375462	-1.34044278348043	-0.10634848196161
C	-0.62447086581501	0.83102322737365	-0.03978139346347
C	1.60385834795871	1.52979173152413	-0.06904919896757
C	-1.05732624177199	2.15867845760945	-0.01089231366487
C	1.22461873705866	2.86929701629985	-0.04072508602992
H	2.65569241462020	1.23173859359291	-0.09290411452293
C	-0.13916778159110	3.22524151722763	-0.01038811277372
H	-2.13067376042035	2.36362671375235	0.01158757911198
H	2.00848615690703	3.62813389477213	-0.04268621505961
C	-1.48747078697437	-0.36158915120203	-0.04266927761879
C	2.88392936937386	-0.36563657291487	-0.01553874376663
C	-3.61000752224278	-1.57119228123815	-0.02066986175762
H	-3.41426373550057	0.58970747260770	0.01026451406004
C	-1.45451993638831	-2.69649333050396	-0.08103189087745
C	-2.84547947321066	-2.75520675820389	-0.05471662476976
H	-0.8425325224459	-3.60232159276041	-0.10780721148562
H	-3.32128593824976	-3.73695749682439	-0.06112053391825
Cl	2.84902396775385	-2.59273926627553	-0.15646579160000
N	0.71400908166937	0.51001102229262	-0.06915199739677
N	-0.76402843686432	-1.53250318803838	-0.07567497621455
C	-0.63203620410991	4.68039948162554	0.02196402700901
C	-5.14633863473835	-1.55803858693969	0.00965773516279
C	-1.46888147197341	4.90906824775261	1.30545260907858
H	-0.86809422441763	4.72512429418277	2.21012183934518
H	-2.34897267495299	4.24863123952838	1.34818073690335
H	-1.83250471909284	5.94906374990897	1.34382088802858
C	-1.51443792393366	4.95000968280246	-1.22245331838395
H	-2.39588355770541	4.29079356649425	-1.25484130454513
H	-0.94674255504053	4.79585198036774	-2.15367068708334
H	-1.87862980694690	5.99048018361612	-1.21396580993006
C	0.53531621483313	5.68677339064346	0.01722584507316
H	1.15609893922674	5.59584772619511	-0.88851929478285
H	1.18817303454198	5.56701319117071	0.89668718239548
H	0.14000136563794	6.71440680030916	0.04093570156401
C	-5.62698575779308	-0.83830419410573	1.29450031730898
H	-5.27505704329918	0.20408534398353	1.34067093863975
H	-5.26555836854063	-1.35397686810619	2.19819210885678
H	-6.72857930512399	-0.81830769015551	1.33148800053130
C	-5.67640647377261	-0.80068838203950	-1.23347184326501
H	-5.35086013281287	-1.28904709250182	-2.16553147250125
H	-5.32589842582464	0.24280972170727	-1.26236114556226
H	-6.77859598588820	-0.78023171481700	-1.22681362251068
C	-5.73745560564246	-2.98142907749125	0.00008283309589
H	-5.42072248600976	-3.56675927917144	0.87820006334712
H	-5.45618808281846	-3.54012746023954	-0.90697506315787
H	-6.83718670287697	-2.92707648033080	0.02271246805954

28

Aryl Acetate Putative Ni(I) Doublet—Phenyl Dissociated

C	4.645468000	0.110289000	-0.075652000
C	3.849233000	1.252747000	-0.027611000
C	4.025680000	-1.145098000	-0.249013000
C	2.642315000	-1.205602000	-0.367861000
N	1.857829000	-0.097579000	-0.363931000
C	2.457940000	1.139153000	-0.179298000
C	1.490717000	2.223492000	-0.159147000
N	0.193938000	1.767603000	0.026352000
C	1.761004000	3.592939000	-0.309458000
H	4.296736000	2.233824000	0.152477000
H	5.729646000	0.185916000	0.038662000
H	4.613314000	-2.064528000	-0.300636000
H	2.105038000	-2.149103000	-0.493656000
C	0.715969000	4.513455000	-0.262353000
H	2.786755000	3.926763000	-0.487354000
C	-0.601651000	4.039956000	-0.090424000
H	0.914550000	5.581968000	-0.375804000
C	-0.818274000	2.672279000	0.029301000
H	-1.448486000	4.728183000	-0.039836000
H	-1.816692000	2.245499000	0.155461000
Ni	-0.008850000	-0.087806000	-0.165343000
O	-0.521630000	-2.014106000	-0.254652000
C	-1.743467000	-1.640678000	-0.152586000
O	-1.984898000	-0.385218000	-0.064177000
C	-2.861432000	-2.648778000	-0.105392000
H	-2.558611000	-3.585903000	-0.590646000
H	-3.764363000	-2.244573000	-0.583078000
H	-3.109648000	-2.870474000	0.945508000