Supporting Information: Theoretical Study

Intermediacy of Ni–Ni Species in sp^2 C–O Bond Cleavage of Aryl Esters: Relevance in Catalytic C–Si Bond Formation

Somerville, Hale, Gómez-Bengoa, Burés, and Martin.

- Computational methods
- Equilibrium between mono- and dinickel species
- Computed catalytic cycle including CsF
- Cartesian coordinates and structures

Computational Methods:

All structures were initially optimized using density functional theory (DFT) by using the B3LYP[1] functional as implemented in Gaussian 09.[2] Optimizations were carried out in a solvent model (IEFPCM, solvent = toluene)[3] by using the 6-31G** basis set for non-metallic atoms and Stuttgart/Dresden (SDD)[4] effective core potential for nickel. The critical stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies, and the intrinsic reaction coordinates (IRC)[5] were followed to verify the energy profiles connecting the key transition structures to the correct associated local minima.

The energies showed in the manuscript have been refined by single-point calculations with the M06[6] functional and def2tzvpp basis set on the previously optimized structures. The values correspond to Free Gibbs energies and are given in kcal/mol. These energies are relative to the [Ni(0)(PCy_3)(naphthyl pivalate)] complex **I**, marked as G = 0.0 kcal/mol in the Figures.

Equilibrium between mono- and dinickel species:

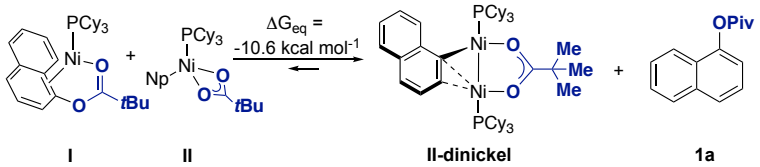


Figure S1: Computed equilibrium between II and II-dinickel. ΔG_{eq} in $kcal/mol^{-1}$

Computed catalytic cycle including CsF:

The catalytic cycle in the absence of fluoride additives is presented in the manuscript. The effect of added CsF in the reaction mechanism was also computed (Figure S2). The same computational method and level as the ones mentioned above were employed, although in this case, the SDD basis set was used for Cs and Ni atoms.

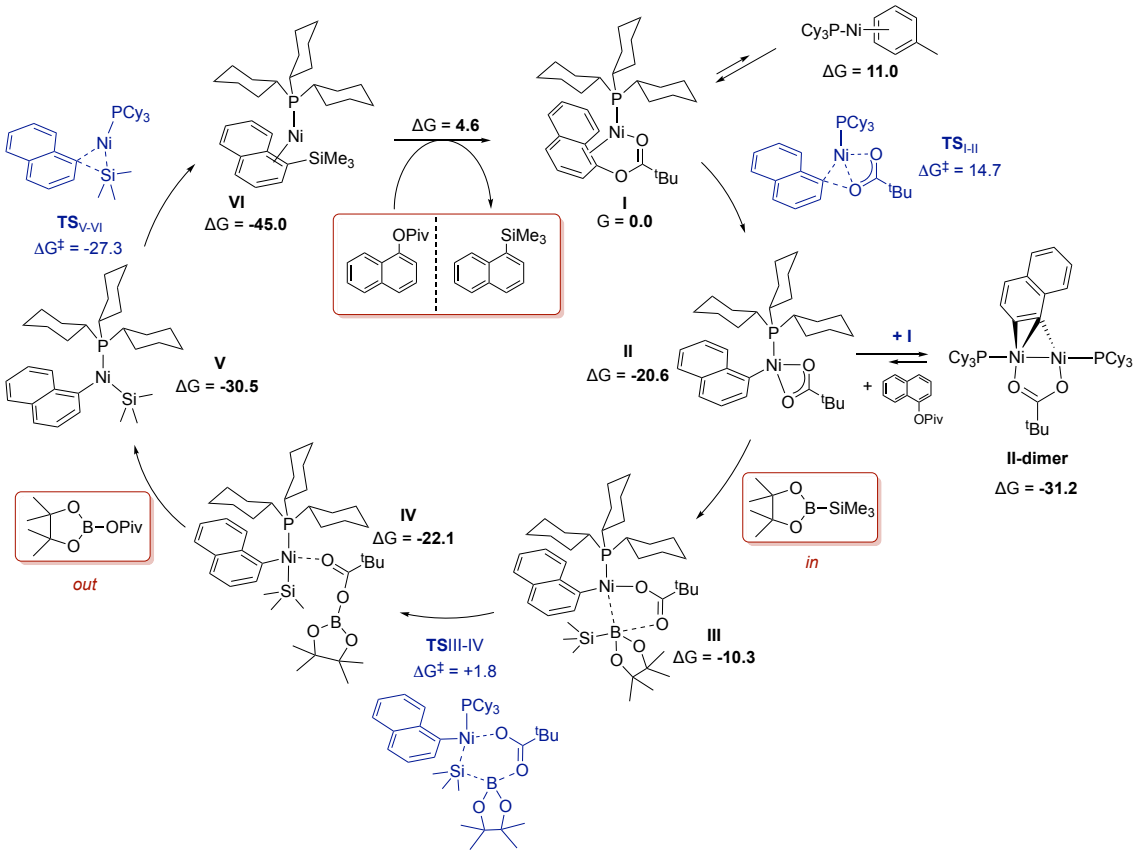


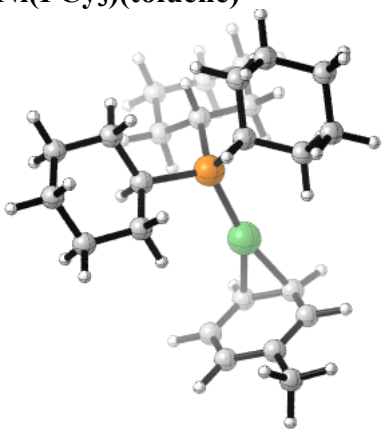
Figure S2: Computed catalytic cycle in the presence of CsF

References

1. (a) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785–789; (b) A. D. Becke, *J. Chem. Phys.*, **1993**, *98*, 5648–5652;
2. Gaussian 09, Revision D.01; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.
3. (a) Cancès, E.; Mennucci, B.; Tomasi, J. *J. Chem. Phys*. **1997**, *107*, 3032–3047. (b) Cossi, M.; Barone, V.; Mennuci, B.; Tomasi, J. *Chem. Phys. Lett.* **1998**, *286*, 253–260. (c) Tomasi, J.; Mennucci, B.; Cancès, E. *J. Mol. Struct. (Theochem)*, **1999**, *464*, 211–226
4. (a) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H.; *J. Chem. Phys*. **1987**, *86*, 866–872. (b) Andrae, D.; Haussermann, U.; Dolg, M.; Stoll H.; Preuss, H.; *Theor. Chim. Acta* **1990**, *77*, 123–141.
5. Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem*. **1990**, *94*, 5523–5527.
6. Zhao, Y.; Truhlar, D. G.; *Theor. Chem. Acc.* **2008**, *120*, 215–241.

Cartesian coordinates of the computed structures:

Ni(PCy_3)(toluene)



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -271.441781 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.548586 Hartrees

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-1.351286	-1.043935	0.037266
2	15	0	0.532405	0.002892	-0.081214
3	6	0	2.009662	-1.101970	-0.489340
4	6	0	2.105344	-2.265938	0.522287
5	6	0	3.276328	-3.211152	0.206533
6	6	0	3.187840	-3.756925	-1.224942
7	6	0	3.089349	-2.613083	-2.243072
8	6	0	1.922501	-1.661550	-1.925920
9	6	0	0.562521	1.310920	-1.449116
10	6	0	1.866334	2.108299	-1.652309
11	6	0	1.766827	3.043033	-2.871855
12	6	0	0.566518	3.993278	-2.756469
13	6	0	-0.738161	3.215748	-2.530571
14	6	0	-0.640152	2.270647	-1.320753
15	6	0	1.050383	0.971212	1.473074
16	6	0	0.366125	0.411755	2.740439
17	6	0	0.629662	1.300296	3.967382
18	6	0	2.131312	1.512621	4.206616
19	6	0	2.820719	2.056315	2.947534
20	6	0	2.562487	1.156617	1.724966
21	1	0	2.925302	-0.500246	-0.412861
22	1	0	2.205438	-1.883490	1.544037
23	1	0	1.161060	-2.827009	0.496742
24	1	0	4.225787	-2.670330	0.330518
25	1	0	3.291735	-4.035642	0.929840
26	1	0	4.053665	-4.392356	-1.447287
27	1	0	2.298354	-4.396859	-1.312654
28	1	0	4.030342	-2.044092	-2.238959
29	1	0	2.973410	-3.013094	-3.257873
30	1	0	1.913813	-0.847571	-2.658789
31	1	0	0.969693	-2.196995	-2.041176
32	1	0	0.388724	0.711595	-2.354031
33	1	0	2.065443	2.717710	-0.760977
34	1	0	2.723368	1.435398	-1.771568
35	1	0	2.697274	3.613795	-2.981068
36	1	0	1.664138	2.436783	-3.783217

37	1	0	0.729982	4.678296	-1.911922
38	1	0	0.488366	4.619069	-3.653750
39	1	0	-1.576635	3.909599	-2.394004
40	1	0	-0.966699	2.624073	-3.428605
41	1	0	-0.537287	2.873488	-0.406833
42	1	0	-1.564199	1.692076	-1.212770
43	1	0	0.620487	1.968226	1.294595
44	1	0	-0.710333	0.310795	2.564191
45	1	0	0.738671	-0.602645	2.939916
46	1	0	0.147158	2.276496	3.813548
47	1	0	0.160468	0.858796	4.855114
48	1	0	2.292357	2.191549	5.052767
49	1	0	2.592358	0.553647	4.483755
50	1	0	2.445890	3.068258	2.736618
51	1	0	3.900587	2.153583	3.114680
52	1	0	3.060365	1.578482	0.846826
53	1	0	3.027841	0.179345	1.906782
54	6	0	-2.856672	-2.133043	-0.810882
55	6	0	-2.931091	-2.135862	0.612526
56	6	0	-3.579155	-1.142180	-1.528928
57	6	0	-3.687544	-1.123092	1.266178
58	1	0	-2.562681	-2.982175	1.188290
59	6	0	-4.346031	-0.196147	-0.863420
60	1	0	-3.555624	-1.151473	-2.615594
61	6	0	-4.403831	-0.164789	0.551521
62	1	0	-3.746091	-1.130810	2.352132
63	1	0	-4.908748	0.538627	-1.434675
64	1	0	-2.425647	-2.974603	-1.346924
65	6	0	-5.234469	0.882099	1.254908
66	1	0	-4.893894	1.895841	1.011381
67	1	0	-6.288881	0.821156	0.958804
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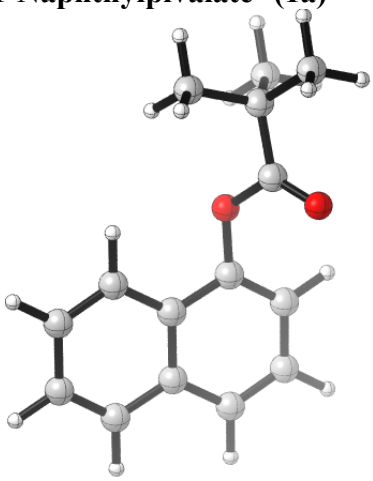
1-Naphthylpivalate (1a)

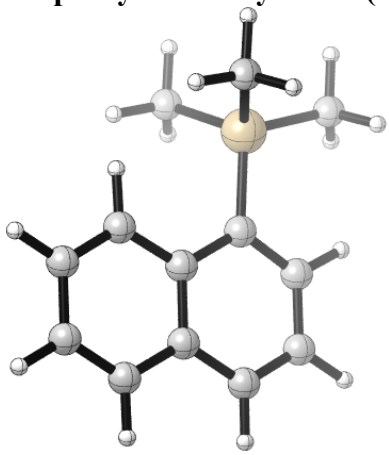


E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -731.460717 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.229920 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.829083	0.043501	0.406126
2	6	0	-2.946567	1.821448	0.036257
3	6	0	-0.542501	2.033089	0.270832

4	6	0	-2.830833	0.406713	-0.001402
5	6	0	-1.828468	2.611752	0.167800
6	6	0	-1.533476	-0.196606	0.094925
7	6	0	-0.409090	0.665269	0.231946
8	1	0	-1.922575	3.692920	0.195560
9	1	0	0.334376	2.660231	0.371601
10	6	0	1.906406	0.393343	-0.376427
11	8	0	1.847932	1.206795	-1.264678
12	6	0	3.159629	-0.374242	0.058688
13	6	0	4.307538	-0.011463	-0.896276
14	1	0	4.504848	1.063339	-0.887105
15	1	0	5.219713	-0.535679	-0.594194
16	1	0	4.071040	-0.293979	-1.925623
17	6	0	3.513354	0.047604	1.503393
18	1	0	3.710375	1.122984	1.564890
19	1	0	2.705115	-0.195049	2.197543
20	1	0	4.417252	-0.477950	1.828407
21	6	0	2.887053	-1.893465	0.012362
22	1	0	2.098976	-2.179131	0.712972
23	1	0	2.591732	-2.214773	-0.991950
24	1	0	3.797944	-2.437395	0.283137
25	6	0	-1.422611	-1.611930	0.053427
26	6	0	-2.545101	-2.397606	-0.078624
27	1	0	-2.447891	-3.478783	-0.111106
28	6	0	-3.828655	-1.807380	-0.172399
29	1	0	-4.705458	-2.439923	-0.274723
30	6	0	-3.965084	-0.438980	-0.134462
31	1	0	-4.948048	0.018808	-0.207033
32	1	0	-3.933458	2.268956	-0.040610
33	1	0	-0.439625	-2.062211	0.126419

1-Naphthyl-trimethylsilane (5a)



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -794.336662 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.208941 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.396622	0.597842	0.000053
2	6	0	0.866593	-0.096456	0.000030
3	6	0	-0.370220	1.985650	0.000219
4	6	0	2.093596	0.651268	-0.000034
5	6	0	0.836910	2.725010	0.000148
6	1	0	-1.302455	2.542861	0.000395

7	6	0	2.043623	2.070507	0.000019
8	1	0	0.800589	3.810738	0.000214
9	14	0	-2.089270	-0.274748	0.000137
10	6	0	-2.302914	-1.336114	-1.557083
11	1	0	-2.239954	-0.714916	-2.457125
12	1	0	-1.544541	-2.119174	-1.647215
13	1	0	-3.285657	-1.821481	-1.557907
14	6	0	-3.461642	1.030930	-0.000516
15	1	0	-4.438699	0.534611	-0.002823
16	1	0	-3.424346	1.672756	0.885863
17	1	0	-3.421102	1.674445	-0.885537
18	6	0	-2.303000	-1.336005	1.557365
19	1	0	-1.546350	-2.120937	1.645818
20	1	0	-2.237001	-0.715436	2.457620
21	1	0	-3.286884	-1.819029	1.559571
22	1	0	2.977679	2.626761	-0.000035
23	6	0	3.336719	-0.036883	-0.000152
24	1	0	4.252803	0.548573	-0.000239
25	6	0	3.387935	-1.411268	-0.000147
26	1	0	4.344777	-1.924931	-0.000241
27	6	0	2.186855	-2.156996	-0.000027
28	1	0	2.227138	-3.242432	0.000002
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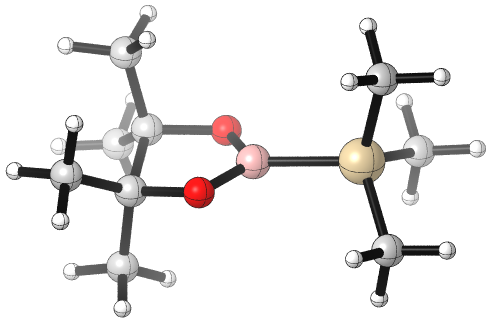
$Me_3SiBpin$



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -820.369279 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.248873 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.332219	0.007195	-0.028641
2	6	0	1.826000	0.786790	0.042331
3	6	0	1.821328	-0.787546	-0.045006
4	8	0	0.432284	-1.076253	-0.391403
5	8	0	0.430573	1.085921	0.351933
6	14	0	-2.364437	0.002871	-0.009882
7	6	0	-3.028612	1.716034	-0.489807
8	1	0	-4.123043	1.746850	-0.439783
9	1	0	-2.639940	2.489763	0.180615
10	1	0	-2.735533	1.987513	-1.509828
11	6	0	-2.969621	-0.419608	1.743884
12	1	0	-4.064894	-0.426743	1.787555
13	1	0	-2.618741	-1.407708	2.060560
14	1	0	-2.613068	0.311300	2.477569
15	6	0	-3.033342	-1.300426	-1.217634

16	1	0	-4.128199	-1.341950	-1.189360
17	1	0	-2.735610	-1.082195	-2.248887
18	1	0	-2.653307	-2.297268	-0.970593
19	6	0	2.086566	-1.477522	1.299250
20	1	0	1.866366	-2.543706	1.199022
21	1	0	3.129881	-1.369039	1.610263
22	1	0	1.445117	-1.073710	2.087188
23	6	0	2.700034	1.376880	1.146914
24	1	0	3.755229	1.134832	0.981656
25	1	0	2.599899	2.465863	1.149226
26	1	0	2.408727	1.010703	2.132758
27	6	0	2.131805	1.474247	-1.294649
28	1	0	1.917530	2.542162	-1.200635
29	1	0	3.181862	1.356890	-1.578633
30	1	0	1.507590	1.074909	-2.098542
31	6	0	2.719378	-1.384381	-1.126553
32	1	0	3.771654	-1.149697	-0.934273
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34	1	0	2.456013	-1.016474	-2.119591

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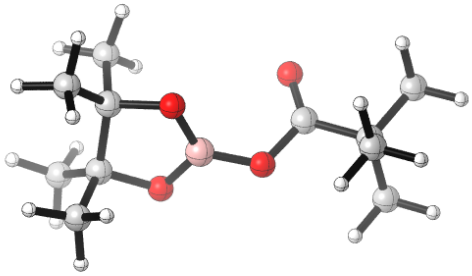
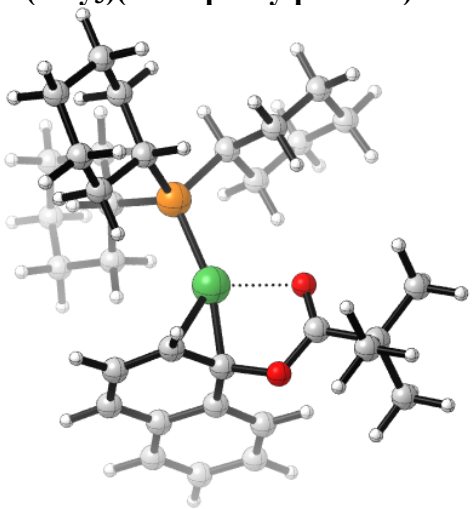


E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -757.562446 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.274532 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.339273	-0.332833	0.016802
2	8	0	1.019024	-0.630140	0.040406
3	6	0	1.952854	0.296782	-0.332457
4	8	0	1.657260	1.291614	-0.952231
5	6	0	3.366086	-0.104267	0.093159
6	6	0	3.405581	-0.214610	1.634082
7	1	0	3.150713	0.739738	2.106562
8	1	0	2.707890	-0.973891	1.995594
9	1	0	4.414388	-0.491352	1.957666
10	6	0	4.354054	0.967516	-0.390733
11	1	0	5.372049	0.695899	-0.093491
12	1	0	4.325898	1.067932	-1.478888
13	1	0	4.117177	1.945382	0.036436
14	6	0	3.708591	-1.473212	-0.536447
15	1	0	3.681060	-1.424033	-1.629982
16	1	0	4.719263	-1.771862	-0.238932
17	1	0	3.009305	-2.246597	-0.210652
18	6	0	-2.296412	0.772459	0.269812
19	6	0	-2.561514	-0.712737	-0.208770
20	8	0	-1.230502	-1.148543	-0.619565
21	8	0	-0.899653	0.716315	0.686565
22	6	0	-2.372226	1.802413	-0.863726

23	1	0	-3.401702	1.955255	-1.200817
24	1	0	-1.981562	2.755954	-0.499783
25	1	0	-1.763136	1.499370	-1.719371
26	6	0	-3.134843	1.230601	1.460006
27	1	0	-2.852642	2.250867	1.734034
28	1	0	-4.200319	1.230672	1.208018
29	1	0	-2.982115	0.593358	2.332613
30	6	0	-3.500616	-0.852559	-1.403448
31	1	0	-3.589859	-1.907426	-1.677626
32	1	0	-4.500585	-0.480798	-1.157399
33	1	0	-3.129366	-0.308422	-2.273069
34	6	0	-2.997912	-1.648723	0.924591
35	1	0	-4.019457	-1.435691	1.252559
36	1	0	-2.959240	-2.680850	0.566413
37	1	0	-2.332286	-1.565287	1.788290

Ni(PCy_3)(κ^2-Naphthylpivalate) I



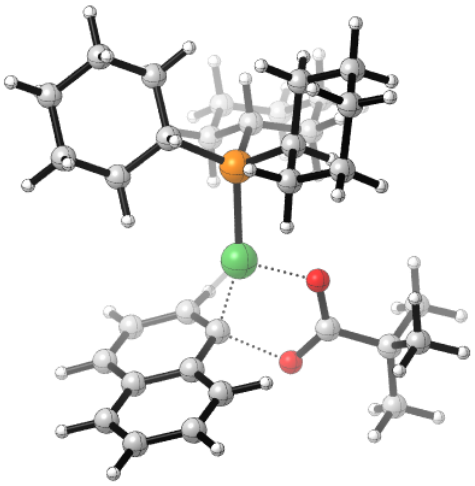
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3286.666269 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.687309 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.072747	2.128317	-2.472990
2	6	0	1.412606	0.780237	-2.097757
3	6	0	2.471642	3.038532	-0.691414
4	6	0	2.337731	0.579504	-1.018962
5	6	0	2.894367	1.726538	-0.308752
6	6	0	1.565695	3.206690	-1.797154
7	6	0	-1.885439	-1.260485	1.571183
8	6	0	-1.828546	-3.608632	2.569250
9	6	0	-1.287510	-1.616752	4.030451
10	6	0	-1.010667	-3.102589	3.765116
11	6	0	-3.236301	3.924026	1.840012
12	6	0	-2.027603	3.927847	0.894047
13	6	0	-2.573488	-1.005102	-1.303598
14	6	0	-4.768035	-1.974759	-2.151963
15	6	0	-3.075450	-1.060523	-3.800761
16	6	0	-4.565982	-1.285981	-3.509109
17	6	0	-2.378361	-0.297069	-2.661415

18	6	0	-4.076054	-1.199267	-1.016212
19	6	0	-4.247910	2.841169	1.439085
20	6	0	-1.047186	-0.765695	2.772381
21	6	0	-1.591343	-2.754807	1.310984
22	6	0	-2.389833	1.456260	0.382920
23	6	0	-1.370041	2.541467	0.796679
24	6	0	-3.589494	1.451932	1.354764
25	6	0	2.988117	4.149308	0.013323
26	1	0	-4.557629	-0.217469	-0.918046
27	1	0	-2.116592	-2.000691	-1.399091
28	1	0	-5.837577	-2.081349	-1.932935
29	1	0	-2.949789	-0.516435	-4.744800
30	1	0	-5.026775	-1.877427	-4.309442
31	1	0	-1.310216	-0.187052	-2.872073
32	1	0	-2.897558	-3.585159	2.826400
33	1	0	-2.329716	-1.494421	4.359287
34	1	0	-4.229455	-1.721404	-0.065152
35	1	0	0.016544	-0.809021	2.502019
36	1	0	-0.547282	-2.863579	0.989117
37	1	0	-2.948804	-1.160298	1.827381
38	1	0	-1.584029	-4.656416	2.355235
39	1	0	-0.657541	-1.250806	4.850349
40	1	0	-1.231776	-3.699080	4.658627
41	1	0	-1.266939	0.284727	2.991451
42	1	0	-2.216581	-3.136058	0.496229
43	1	0	0.059323	-3.237456	3.553268
44	1	0	1.288096	-0.006360	-2.840600
45	1	0	-4.682165	3.094609	0.461150
46	1	0	-2.354629	4.240295	-0.108466
47	1	0	-2.892000	3.732769	2.866647
48	1	0	-0.931643	2.281039	1.769956
49	1	0	-3.249283	1.166846	2.358362
50	1	0	-2.769874	1.740874	-0.609791
51	1	0	-5.081805	2.812642	2.151422
52	1	0	-1.286810	4.666490	1.222772
53	1	0	-3.718041	4.909302	1.851797
54	1	0	-0.542181	2.565140	0.081609
55	1	0	-4.335734	0.709132	1.057098
56	1	0	0.413751	2.275253	-3.325651
57	1	0	-4.355907	-2.993005	-2.196139
58	1	0	-2.582048	-2.033990	-3.934013
59	1	0	-5.083480	-0.315880	-3.500807
60	1	0	-2.792149	0.720011	-2.610009
61	8	0	3.237162	-0.577524	-1.073767
62	15	0	-1.526349	-0.201700	0.049755
63	28	0	0.628968	-0.018733	-0.412396
64	6	0	2.878239	-1.613224	-0.316933
65	8	0	1.827312	-1.624592	0.330526
66	6	0	3.874114	-2.771913	-0.352412
67	6	0	3.994609	-3.267983	-1.812708
68	1	0	4.359466	-2.476682	-2.471618
69	1	0	4.696063	-4.107644	-1.856907
70	1	0	3.028795	-3.616792	-2.193686
71	6	0	5.249369	-2.265502	0.138858
72	1	0	5.195559	-1.913183	1.174566
73	1	0	5.975584	-3.084115	0.102336
74	1	0	5.617000	-1.447536	-0.484948
75	6	0	3.370687	-3.907594	0.552142
76	1	0	3.265676	-3.574548	1.588150
77	1	0	2.396551	-4.276830	0.220846

78	1	0	4.081908	-4.739490	0.527222
79	6	0	3.833317	1.591308	0.735706
80	6	0	3.895346	3.990054	1.046803
81	6	0	4.324658	2.700631	1.406509
82	1	0	5.042708	2.571352	2.211500
83	1	0	4.176541	0.600575	1.015085
84	1	0	4.279971	4.858679	1.573827
85	1	0	2.664156	5.145187	-0.279952
86	1	0	1.292640	4.216535	-2.091307

TS_{I-II}



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3286.639148 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.683534 Hartrees
Imaginary frequency: -182.142

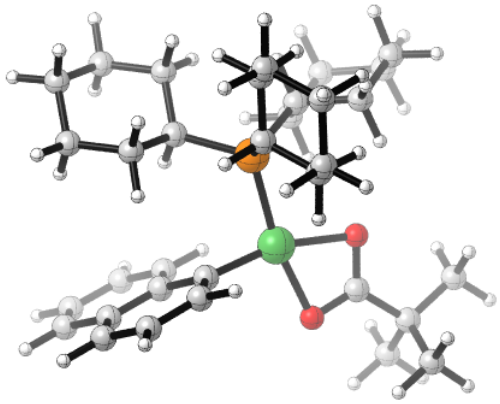
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.382538	2.875337	-0.381776
2	6	0	-3.177268	1.519294	0.034480
3	6	0	-2.034845	2.518094	-2.382510
4	6	0	-2.332293	0.681941	-0.784103
5	6	0	-1.800311	1.163439	-1.993674
6	6	0	-2.794985	3.346757	-1.599713
7	6	0	2.602399	-0.691936	-1.304330
8	6	0	3.118553	-2.747776	-2.727574
9	6	0	3.225323	-0.446061	-3.769600
10	6	0	2.921767	-1.930528	-4.011385
11	6	0	3.577702	4.346565	0.322638
12	6	0	2.071972	4.184758	0.574983
13	6	0	1.863235	-1.141736	1.542555
14	6	0	3.438442	-2.403005	3.087582
15	6	0	1.114905	-1.781848	3.889658
16	6	0	2.575340	-2.021290	4.298837
17	6	0	1.000123	-0.743287	2.760566
18	6	0	3.330123	-1.355303	1.964968
19	6	0	4.364082	3.147242	0.870221
20	6	0	2.393071	0.115752	-2.605322
21	6	0	2.295627	-2.185718	-1.555182
22	6	0	2.327222	1.649542	0.586031
23	6	0	1.538541	2.852917	0.022296

24	6	0	3.836161	1.816180	0.305192
25	1	0	3.748538	-0.407137	2.328267
26	1	0	1.465643	-2.100116	1.181519
27	1	0	4.486986	-2.521191	3.387034
28	1	0	0.525112	-1.455701	4.754694
29	1	0	2.633419	-2.801119	5.067570
30	1	0	-0.045875	-0.633556	2.455445
31	1	0	4.183857	-2.741783	-2.455257
32	1	0	4.294712	-0.325005	-3.544529
33	1	0	3.943485	-1.661591	1.109437
34	1	0	1.328201	0.085883	-2.872497
35	1	0	1.224217	-2.303743	-1.767557
36	1	0	3.656950	-0.604455	-1.010205
37	1	0	2.847501	-3.796884	-2.896445
38	1	0	3.030820	0.137443	-4.677566
39	1	0	3.554979	-2.324812	-4.815070
40	1	0	2.639918	1.171675	-2.450398
41	1	0	2.499837	-2.777456	-0.656608
42	1	0	1.881815	-2.035694	-4.351719
43	1	0	-1.349704	0.479824	-2.709102
44	1	0	4.284591	3.130483	1.966605
45	1	0	1.880166	4.226488	1.656891
46	1	0	3.756494	4.431070	-0.758948
47	1	0	1.610365	2.858594	-1.073767
48	1	0	4.012606	1.801492	-0.777893
49	1	0	2.192755	1.665059	1.677741
50	1	0	5.431015	3.250388	0.637513
51	1	0	1.517385	5.019103	0.129567
52	1	0	3.942930	5.277778	0.771978
53	1	0	0.473637	2.745917	0.254576
54	1	0	4.408458	0.983358	0.725740
55	1	0	3.111885	-3.379076	2.701584
56	1	0	0.672341	-2.728650	3.549521
57	1	0	2.978658	-1.104838	4.753343
58	1	0	1.325673	0.234094	3.144494
59	8	0	-3.233462	-1.047765	-0.914727
60	15	0	1.537898	0.003299	0.084642
61	28	0	-0.694082	0.075182	-0.347300
62	6	0	-2.514228	-1.917235	-0.340666
63	8	0	-1.343374	-1.698593	0.118039
64	6	0	-3.069699	-3.348423	-0.187036
65	6	0	-3.007046	-3.740342	1.304530
66	1	0	-3.639915	-3.084996	1.913114
67	1	0	-3.366915	-4.766877	1.435644
68	1	0	-1.984700	-3.676961	1.684068
69	6	0	-4.517666	-3.436408	-0.694619
70	1	0	-4.586245	-3.164260	-1.750830
71	1	0	-4.891096	-4.459597	-0.575036
72	1	0	-5.174625	-2.762551	-0.138129
73	6	0	-2.162516	-4.290903	-1.008623
74	1	0	-2.181431	-4.028812	-2.072160
75	1	0	-1.128172	-4.240223	-0.659534
76	1	0	-2.513129	-5.324309	-0.911995
77	6	0	-3.779700	1.070165	1.232705
78	6	0	-4.175835	3.721418	0.434336
79	6	0	-4.751591	3.256426	1.599190
80	1	0	-5.360013	3.919599	2.207911
81	6	0	-4.554786	1.918009	2.000542
82	1	0	-5.014801	1.554405	2.915018
83	1	0	-1.621405	2.878076	-3.321667

84	1	0	-2.979607	4.375046	-1.899147
85	1	0	-4.329717	4.751019	0.119972
86	1	0	-3.632758	0.038659	1.533910

II-monomer

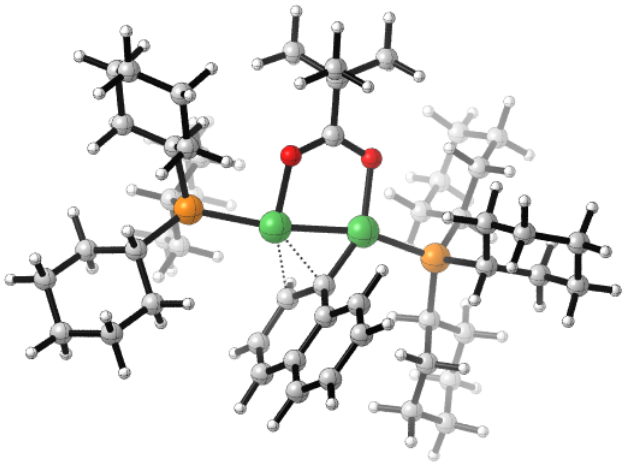


E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3286.700904 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.689040 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.811738	-3.185584	0.604595
2	6	0	1.662347	-2.493230	0.086175
3	6	0	2.340869	-2.297192	2.810762
4	6	0	0.865337	-1.674493	0.953861
5	6	0	1.217607	-1.601557	2.292262
6	6	0	3.128580	-3.064659	1.984374
7	6	0	-0.800441	2.059755	-1.336690
8	6	0	-1.819342	1.985740	-3.674876
9	6	0	-2.897024	3.391573	-1.871037
10	6	0	-3.138462	2.550181	-3.131175
11	6	0	-0.111622	4.140854	3.551950
12	6	0	-0.475628	2.664435	3.764461
13	6	0	1.951658	0.985177	-0.900282
14	6	0	3.661928	1.782122	-2.600846
15	6	0	4.427996	0.520523	-0.547323
16	6	0	4.797485	1.585126	-1.588729
17	6	0	3.089287	0.840625	0.138701
18	6	0	2.318467	2.093364	-1.914567
19	6	0	1.074694	4.286178	2.588955
20	6	0	-2.137219	2.605003	-0.786496
21	6	0	-1.062878	1.195027	-2.594443
22	6	0	0.438235	2.096621	1.460187
23	6	0	-0.757053	1.951340	2.431029
24	6	0	0.811516	3.578949	1.247048
25	1	0	2.392027	3.062750	-1.404029
26	1	0	1.905234	0.037575	-1.451913
27	1	0	3.908553	2.588156	-3.302631
28	1	0	5.215221	0.437864	0.211429
29	1	0	5.724085	1.311001	-2.107007
30	1	0	2.853215	0.061300	0.865767
31	1	0	-1.188288	2.811994	-4.033711
32	1	0	-2.319863	4.288426	-2.140461
33	1	0	1.549873	2.202589	-2.683868

34	1	0	-2.753095	1.772368	-0.433300
35	1	0	-1.661245	0.325753	-2.297484
36	1	0	-0.186563	2.922488	-1.627947
37	1	0	-2.006666	1.338906	-4.540366
38	1	0	-3.850171	3.747528	-1.461814
39	1	0	-3.643005	3.149527	-3.898546
40	1	0	-1.960552	3.265389	0.067498
41	1	0	-0.124732	0.807932	-3.008943
42	1	0	-3.812340	1.717755	-2.886156
43	1	0	0.625145	-1.001666	2.980415
44	1	0	1.972230	3.853210	3.052805
45	1	0	0.353944	2.157720	4.277860
46	1	0	-0.980806	4.673339	3.139849
47	1	0	-1.664064	2.372916	1.983712
48	1	0	-0.002347	4.096471	0.723767
49	1	0	1.290732	1.602882	1.945620
50	1	0	1.296656	5.345141	2.410208
51	1	0	-1.349002	2.576404	4.421369
52	1	0	0.119311	4.618234	4.511565
53	1	0	-0.966330	0.890140	2.606003
54	1	0	1.696486	3.663928	0.608162
55	1	0	3.549829	0.868799	-3.201678
56	1	0	4.356373	-0.463127	-1.029996
57	1	0	4.995576	2.538673	-1.078053
58	1	0	3.196907	1.782014	0.694404
59	8	0	-1.909971	-2.431303	0.657932
60	15	0	0.227997	1.075204	-0.103039
61	28	0	-0.732498	-0.875160	0.352012
62	6	0	-2.901161	-1.735823	0.260103
63	8	0	-2.667919	-0.534113	-0.108803
64	6	0	-4.306869	-2.333033	0.250302
65	6	0	-5.311473	-1.347685	-0.365605
66	1	0	-5.047995	-1.105762	-1.399378
67	1	0	-6.314255	-1.788415	-0.361804
68	1	0	-5.345177	-0.410663	0.196742
69	6	0	-4.267136	-3.645795	-0.562062
70	1	0	-3.532366	-4.338820	-0.145942
71	1	0	-5.251905	-4.125030	-0.544317
72	1	0	-4.003930	-3.455940	-1.608384
73	6	0	-4.687743	-2.644687	1.716163
74	1	0	-3.962166	-3.324480	2.169789
75	1	0	-4.725790	-1.730124	2.318004
76	1	0	-5.676945	-3.113869	1.752523
77	6	0	1.357385	-2.653663	-1.296166
78	6	0	3.598973	-3.977459	-0.276183
79	6	0	3.275410	-4.097879	-1.609008
80	1	0	3.887010	-4.709769	-2.266402
81	6	0	2.137874	-3.430858	-2.124516
82	1	0	1.878425	-3.539735	-3.174045
83	1	0	4.466490	-4.495375	0.126803
84	1	0	3.995733	-3.592397	2.373932
85	1	0	2.578164	-2.215582	3.868983
86	1	0	0.475467	-2.152645	-1.688382

II-dinickel



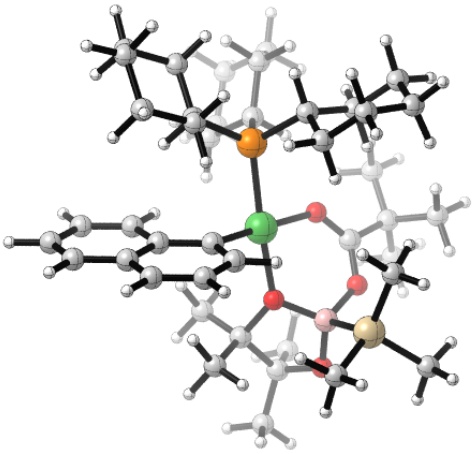
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -5841.922968 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 1.146128 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.083068	3.718425	-1.132780
2	6	0	4.082048	-1.441422	1.329429
3	6	0	0.503371	2.425616	-1.314100
4	6	0	-0.846708	3.090710	1.088606
5	6	0	0.464424	1.428162	-0.242510
6	6	0	-0.299969	1.770022	0.909772
7	6	0	-0.725843	4.034628	0.113197
8	6	0	-3.793014	-0.496598	2.010169
9	6	0	-3.458705	-2.298649	3.780850
10	6	0	-3.547279	0.136794	4.467994
11	6	0	-2.962811	-1.247191	4.783538
12	6	0	-6.195186	3.995196	0.116124
13	6	0	-4.947953	3.887518	-0.772396
14	6	0	-4.189247	-1.369977	-0.801229
15	6	0	-6.103858	-2.955346	-1.355505
16	6	0	-4.464503	-2.292174	-3.164593
17	6	0	-5.916229	-2.681700	-2.853956
18	6	0	-3.991503	-1.102447	-2.310530
19	6	0	-5.652952	-1.754312	-0.505002
20	6	0	-6.878459	2.630160	0.276296
21	6	0	-3.256917	0.547110	3.015158
22	6	0	-3.186230	-1.881694	2.324965
23	6	0	-4.665676	1.442963	-0.129572
24	6	0	-3.975120	2.812470	-0.261393
25	6	0	-5.900566	1.557918	0.791482
26	1	0	-6.312840	-0.906459	-0.730714
27	1	0	-3.547246	-2.221784	-0.551631
28	1	0	-7.152660	-3.191971	-1.137365
29	1	0	-4.352962	-2.050675	-4.228761
30	1	0	-6.210507	-3.559356	-3.442185
31	1	0	-2.936610	-0.890973	-2.509945
32	1	0	-4.540093	-2.444586	3.916871
33	1	0	-4.634329	0.119442	4.632206
34	1	0	-5.789163	-1.984402	0.557911
35	1	0	-2.172872	0.645714	2.880179
36	1	0	-2.103132	-1.848447	2.145352
37	1	0	-4.880878	-0.566537	2.142786

38	1	0	-2.987615	-3.268624	3.981506
39	1	0	-3.140652	0.889053	5.154973
40	1	0	-3.217804	-1.546726	5.807282
41	1	0	-3.683267	1.536009	2.814464
42	1	0	-3.587837	-2.643161	1.648430
43	1	0	-1.865717	-1.193057	4.737127
44	1	0	-0.186452	1.168425	1.813695
45	1	0	-7.282510	2.310908	-0.695201
46	1	0	-5.255036	3.638246	-1.798662
47	1	0	-5.901607	4.369535	1.107542
48	1	0	-3.579476	3.118765	0.714172
49	1	0	-5.582830	1.830584	1.805856
50	1	0	-5.037754	1.182296	-1.130267
51	1	0	-7.734289	2.707869	0.958238
52	1	0	-4.434221	4.854761	-0.829520
53	1	0	-6.899887	4.727230	-0.296731
54	1	0	-3.109716	2.737842	-0.926043
55	1	0	-6.422687	0.600478	0.875843
56	1	0	-5.518437	-3.841413	-1.071441
57	1	0	-3.813208	-3.155333	-2.971418
58	1	0	-6.585665	-1.863649	-3.157483
59	1	0	-4.560669	-0.211901	-2.612798
60	15	0	-3.443165	0.025760	0.228967
61	28	0	-1.099877	0.100601	-0.158427
62	6	0	-0.075863	-2.516893	-0.877874
63	6	0	-0.294520	-3.952215	-1.407976
64	6	0	-0.578217	-3.841159	-2.923763
65	1	0	0.276981	-3.406104	-3.452248
66	1	0	-0.765641	-4.834720	-3.346606
67	1	0	-1.451202	-3.212330	-3.114140
68	6	0	0.955178	-4.818472	-1.181679
69	1	0	1.190250	-4.908159	-0.116707
70	1	0	0.784644	-5.825883	-1.578093
71	1	0	1.829208	-4.394250	-1.681005
72	6	0	-1.501033	-4.596764	-0.697999
73	1	0	-1.337105	-4.661693	0.383379
74	1	0	-2.414103	-4.023700	-0.868832
75	1	0	-1.658239	-5.613830	-1.074475
76	6	0	3.678987	-2.790835	3.461201
77	6	0	4.738157	-3.899245	1.450215
78	6	0	3.844080	-4.101780	2.681136
79	6	0	6.490022	-0.451077	-3.355874
80	6	0	4.981118	-0.356894	-3.624495
81	6	0	3.704502	1.499752	1.410639
82	6	0	4.875091	2.713767	3.310577
83	6	0	3.663527	4.042053	1.527066
84	6	0	4.829525	4.031706	2.525295
85	6	0	3.704765	2.815123	0.601729
86	6	0	4.906580	1.485659	2.381030
87	6	0	6.896775	0.440731	-2.174762
88	6	0	4.226914	-2.763795	0.545708
89	6	0	3.164916	-1.659016	2.556657
90	6	0	4.563517	0.213611	-1.178301
91	6	0	4.161139	-0.690330	-2.367368
92	6	0	6.080582	0.122510	-0.908197
93	1	0	5.846986	1.490715	1.815085
94	1	0	2.791402	1.504754	2.022317
95	1	0	5.746726	2.694916	3.976469
96	1	0	3.683252	4.958559	0.925327
97	1	0	4.754641	4.881783	3.214263

98	1	0	2.858514	2.841501	-0.089054
99	1	0	4.647605	-2.500493	3.893676
100	1	0	5.760830	-3.667072	1.782269
101	1	0	4.915557	0.577978	2.991567
102	1	0	3.256907	-3.035529	0.115936
103	1	0	2.158136	-1.906776	2.195900
104	1	0	5.079615	-1.151745	1.687562
105	1	0	2.991823	-2.930929	4.304651
106	1	0	4.804129	-4.828123	0.870540
107	1	0	4.257537	-4.883721	3.329757
108	1	0	4.923169	-2.638231	-0.288826
109	1	0	3.067811	-0.736646	3.140702
110	1	0	2.855075	-4.453691	2.355406
111	1	0	6.738862	1.494098	-2.447063
112	1	0	4.736044	0.661999	-3.957180
113	1	0	6.752277	-1.494558	-3.128805
114	1	0	4.315878	-1.744425	-2.110098
115	1	0	6.337268	-0.887614	-0.563102
116	1	0	4.342892	1.244439	-1.488844
117	1	0	7.967417	0.331277	-1.962477
118	1	0	4.695951	-1.029457	-4.442572
119	1	0	7.057044	-0.175202	-4.253090
120	1	0	3.090277	-0.582846	-2.569720
121	1	0	6.372335	0.808446	-0.106720
122	1	0	3.988364	2.647604	3.957242
123	1	0	2.709592	4.048176	2.072046
124	1	0	5.774526	4.157048	1.976953
125	1	0	4.618477	2.867947	-0.006214
126	15	0	3.409931	-0.012438	0.298953
127	28	0	1.250751	-0.232593	-0.241456
128	8	0	1.099965	-2.174150	-0.554727
129	8	0	-1.094352	-1.749909	-0.833339
130	6	0	-0.009687	4.666508	-2.181438
131	6	0	0.619685	4.366103	-3.375659
132	6	0	1.202434	3.097100	-3.560045
133	6	0	1.143633	2.155141	-2.546697
134	1	0	1.581957	1.170950	-2.685216
135	1	0	1.691289	2.855954	-4.500091
136	1	0	0.662749	5.105337	-4.170896
137	1	0	-0.462901	5.644358	-2.033482
138	1	0	-1.124357	5.036996	0.252151
139	1	0	-1.329810	3.338416	2.031667

III



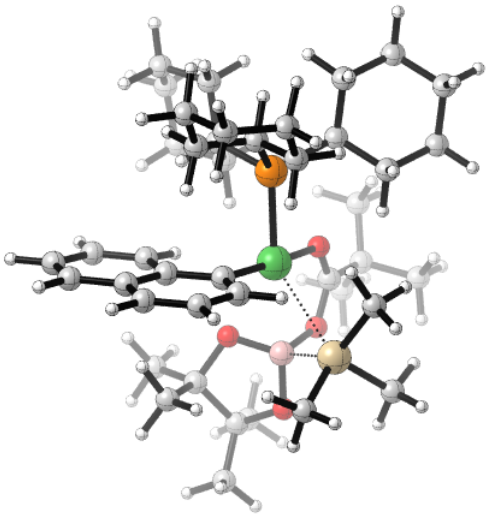
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -4107.084449 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.968685 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.821119	4.072292	0.286830
2	6	0	-1.422231	2.827553	-0.322203
3	6	0	-0.567318	3.504687	2.278443
4	6	0	-0.578136	1.915635	0.400028
5	6	0	-0.177480	2.282291	1.677264
6	6	0	-1.375926	4.384662	1.597677
7	6	0	-1.723078	-2.006091	1.671477
8	6	0	-0.948786	-4.174676	2.756984
9	6	0	-1.311899	-2.124179	4.187425
10	6	0	-0.523522	-3.430198	4.028459
11	6	0	-6.088976	0.971442	1.234306
12	6	0	-4.807476	1.712635	1.630763
13	6	0	-1.889390	-2.060566	-1.338481
14	6	0	-2.668274	-4.165500	-2.514401
15	6	0	-1.788275	-2.219735	-3.877974
16	6	0	-2.758066	-3.408952	-3.847645
17	6	0	-1.977986	-1.282553	-2.671470
18	6	0	-2.912107	-3.222223	-1.321790
19	6	0	-5.905009	0.268115	-0.114242
20	6	0	-1.226960	-1.248139	2.925834
21	6	0	-0.858029	-3.277362	1.510318
22	6	0	-3.388253	0.087401	0.269264
23	6	0	-3.595113	0.766710	1.643974
24	6	0	-4.677132	-0.663146	-0.133834
25	1	0	-3.933741	-2.842814	-1.393286
26	1	0	-0.888505	-2.504848	-1.309108
27	1	0	-3.397791	-4.983968	-2.490344
28	1	0	-1.909273	-1.651779	-4.808214
29	1	0	-2.553534	-4.085453	-4.685802
30	1	0	-1.211902	-0.499762	-2.699466
31	1	0	-1.982586	-4.532168	2.869653
32	1	0	-2.366380	-2.355405	4.397288
33	1	0	-2.861286	-3.785318	-0.385475
34	1	0	-0.184640	-0.956973	2.755778
35	1	0	0.181576	-2.973173	1.351271
36	1	0	-2.766526	-2.316722	1.833104
37	1	0	-0.327416	-5.066431	2.609902

38	1	0	-0.940336	-1.557197	5.048942
39	1	0	-0.657306	-4.069534	4.909111
40	1	0	-1.782394	-0.324779	3.088309
41	1	0	-1.149687	-3.856142	0.631768
42	1	0	0.548232	-3.196298	3.969641
43	1	0	0.473818	1.624925	2.246074
44	1	0	-5.782852	1.026349	-0.900329
45	1	0	-4.620167	2.533562	0.926247
46	1	0	-6.332459	0.226373	2.005591
47	1	0	-3.771408	-0.004340	2.405298
48	1	0	-4.849962	-1.512180	0.542113
49	1	0	-3.240633	0.888104	-0.462049
50	1	0	-6.799848	-0.309950	-0.375381
51	1	0	-4.918298	2.170547	2.620867
52	1	0	-6.938317	1.663445	1.189084
53	1	0	-2.701720	1.320656	1.936810
54	1	0	-4.582354	-1.070798	-1.141150
55	1	0	-1.675535	-4.627234	-2.421228
56	1	0	-0.756021	-2.596141	-3.874650
57	1	0	-3.786039	-3.043907	-3.985038
58	1	0	-2.951139	-0.779347	-2.752531
59	15	0	-1.764200	-0.890175	0.141273
60	28	0	0.192895	0.267326	-0.169041
61	5	0	3.225006	0.536536	0.112884
62	8	0	3.255461	-1.006605	-0.269505
63	6	0	2.294537	-1.793683	-0.569304
64	8	0	1.067884	-1.491616	-0.572799
65	6	0	2.742418	-3.230786	-0.914493
66	6	0	3.241490	-3.885258	0.395921
67	1	0	3.593989	-4.901696	0.190432
68	1	0	4.067156	-3.313488	0.826539
69	1	0	2.442426	-3.952593	1.142004
70	6	0	1.593143	-4.056542	-1.509279
71	1	0	1.954763	-5.058802	-1.762466
72	1	0	0.765238	-4.164930	-0.805493
73	1	0	1.205187	-3.598441	-2.424236
74	6	0	3.909337	-3.167427	-1.923364
75	1	0	3.591154	-2.723320	-2.872687
76	1	0	4.736625	-2.573825	-1.530914
77	1	0	4.270291	-4.180166	-2.132397
78	14	0	3.663637	0.660004	2.131209
79	6	0	2.589276	-0.348066	3.353415
80	1	0	3.066693	-0.385606	4.340392
81	1	0	1.594815	0.088840	3.494294
82	1	0	2.455245	-1.383092	3.016920
83	6	0	3.666389	2.462610	2.757101
84	1	0	4.362110	3.071826	2.169434
85	1	0	2.677089	2.926665	2.681467
86	1	0	3.984029	2.517875	3.805513
87	6	0	5.441364	-0.001635	2.333734
88	1	0	5.496138	-1.072597	2.106360
89	1	0	6.117990	0.512632	1.643740
90	1	0	5.817517	0.141915	3.353929
91	8	0	1.987218	1.099396	-0.528386
92	8	0	4.312020	1.170408	-0.570642
93	6	0	2.381503	2.113873	-1.520214
94	6	0	3.875686	1.716837	-1.815848
95	6	0	1.454224	2.021480	-2.728453
96	1	0	0.431211	2.189290	-2.396523
97	1	0	1.708543	2.785665	-3.470268

98	1	0	1.503169	1.041516	-3.207657
99	6	0	2.259001	3.492625	-0.860492
100	1	0	2.530614	4.287602	-1.561780
101	1	0	1.230851	3.659265	-0.538269
102	1	0	2.907918	3.562784	0.015094
103	6	0	4.786921	2.902166	-2.152620
104	1	0	5.800187	2.532888	-2.337078
105	1	0	4.448658	3.427379	-3.052630
106	1	0	4.835930	3.612478	-1.326131
107	6	0	4.021226	0.655644	-2.923704
108	1	0	3.835058	1.074942	-3.918299
109	1	0	5.044836	0.272019	-2.898643
110	1	0	3.344942	-0.186933	-2.771676
111	6	0	-1.898851	2.569732	-1.642388
112	1	0	-1.615363	1.636078	-2.117210
113	6	0	-2.655776	4.969736	-0.437201
114	1	0	-2.943370	5.904165	0.039306
115	6	0	-3.090467	4.676784	-1.709059
116	1	0	-3.724238	5.376085	-2.247008
117	6	0	-2.705777	3.458421	-2.318610
118	1	0	-3.047094	3.225992	-3.323686
119	1	0	-0.218058	3.742446	3.280126
120	1	0	-1.681099	5.326252	2.047179

$TS_{III\text{-}IV}$



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -4107.066405 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.969868 Hartrees
Imaginary Frequency: -72.9

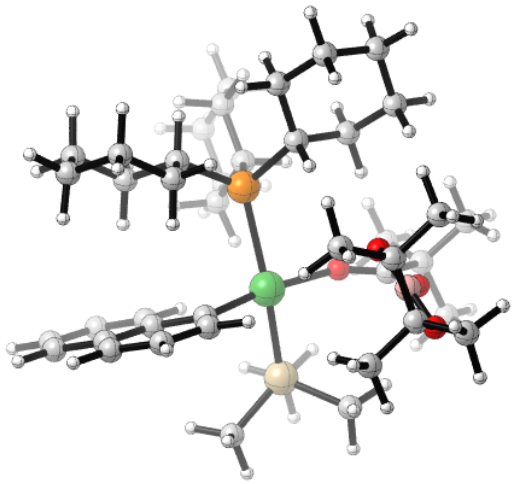
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.086328	-4.189292	-0.069826
2	6	0	-0.086784	-2.789546	0.223345
3	6	0	0.295345	-3.667367	-2.421524
4	6	0	-0.049659	-1.811492	-0.836613
5	6	0	0.145513	-2.288272	-2.125230
6	6	0	0.275850	-4.602626	-1.414754
7	6	0	3.341710	-0.788715	-0.670863
8	6	0	4.579058	-3.002017	-0.780725
9	6	0	4.584942	-1.464142	-2.787352
10	6	0	4.621709	-2.923012	-2.312258
11	6	0	3.916795	4.426178	-1.480337
12	6	0	2.402281	4.199373	-1.571563
13	6	0	2.191845	-0.027499	1.949008
14	6	0	3.630860	-0.391514	4.007488
15	6	0	1.223783	0.346009	4.270769
16	6	0	2.635789	0.397227	4.869271
17	6	0	1.202625	0.798591	2.799734
18	6	0	3.611839	0.090694	2.545328
19	6	0	4.494631	3.758193	-0.226392
20	6	0	3.374476	-0.706491	-2.212971
21	6	0	3.354932	-2.263126	-0.211629
22	6	0	2.598424	2.059125	-0.200550
23	6	0	2.031315	2.708824	-1.482712
24	6	0	4.132527	2.263308	-0.162945
25	1	0	3.933882	1.138840	2.525128
26	1	0	1.885156	-1.077905	2.033867
27	1	0	4.645797	-0.298048	4.412343
28	1	0	0.537212	0.967971	4.857633
29	1	0	2.629328	0.010928	5.895341
30	1	0	0.188473	0.717404	2.399150
31	1	0	5.499694	-2.564513	-0.367102
32	1	0	5.510527	-0.958036	-2.476148
33	1	0	4.341348	-0.479028	1.960946
34	1	0	2.451895	-1.139423	-2.612109

35	1	0	2.446372	-2.763372	-0.551938
36	1	0	4.267253	-0.328878	-0.299763
37	1	0	4.555754	-4.047851	-0.452708
38	1	0	4.558788	-1.417301	-3.882664
39	1	0	5.516896	-3.425783	-2.697540
40	1	0	3.408300	0.334751	-2.547731
41	1	0	3.364286	-2.334823	0.880473
42	1	0	3.755511	-3.459688	-2.722440
43	1	0	0.180672	-1.597097	-2.959819
44	1	0	4.107037	4.263226	0.669830
45	1	0	1.908046	4.744192	-0.754705
46	1	0	4.402263	4.001652	-2.370581
47	1	0	2.425291	2.193761	-2.367553
48	1	0	4.590263	1.759666	-1.023835
49	1	0	2.161510	2.597350	0.650694
50	1	0	5.585243	3.870998	-0.199536
51	1	0	2.008460	4.618670	-2.505327
52	1	0	4.145283	5.498594	-1.482180
53	1	0	0.948706	2.596308	-1.506909
54	1	0	4.577716	1.819355	0.729926
55	1	0	3.378213	-1.460467	4.039455
56	1	0	0.842607	-0.682600	4.331300
57	1	0	2.965686	1.444287	4.931775
58	1	0	1.472591	1.861726	2.745251
59	15	0	1.986698	0.279886	0.093383
60	28	0	-0.254512	0.048997	-0.443277
61	14	0	-2.152172	0.450295	-2.499985
62	5	0	-2.903185	0.424821	-0.367458
63	6	0	-0.513778	0.945707	-3.389378
64	1	0	0.398842	0.422853	-3.096962
65	1	0	-0.663089	0.781216	-4.465258
66	1	0	-0.337676	2.017207	-3.251100
67	6	0	-3.261205	1.906408	-3.062792
68	1	0	-4.290178	1.771844	-2.725338
69	1	0	-2.898989	2.866869	-2.680710
70	1	0	-3.251083	1.964411	-4.158914
71	6	0	-2.850402	-1.095920	-3.359433
72	1	0	-2.778481	-0.983569	-4.448470
73	1	0	-2.336782	-2.019001	-3.081521
74	1	0	-3.907792	-1.197936	-3.099408
75	8	0	-2.750025	1.894333	0.131671
76	6	0	-1.627456	2.454231	0.385270
77	8	0	-0.509140	1.913722	0.175259
78	6	0	-1.709434	3.895977	0.911926
79	6	0	-0.415798	4.287607	1.642320
80	1	0	-0.487819	5.324934	1.985165
81	1	0	-0.246146	3.654413	2.518474
82	1	0	0.454585	4.202687	0.989035
83	6	0	-1.915371	4.810938	-0.320738
84	1	0	-1.079440	4.729284	-1.023185
85	1	0	-2.837918	4.556493	-0.849496
86	1	0	-1.982493	5.854787	0.003852
87	6	0	-2.912183	4.040449	1.865250
88	1	0	-2.803036	3.393179	2.741934
89	1	0	-2.978695	5.075217	2.217603
90	1	0	-3.847543	3.780810	1.366782
91	6	0	-4.952814	-0.424115	0.318647
92	6	0	-3.804919	-1.284133	0.967602
93	8	0	-4.264603	0.243772	-0.756497
94	8	0	-2.628176	-0.468094	0.722981

95	6	0	-5.520070	0.645722	1.268221
96	1	0	-6.142271	1.333613	0.688215
97	1	0	-6.139684	0.201481	2.054464
98	1	0	-4.723472	1.226784	1.736684
99	6	0	-3.937989	-1.493828	2.477539
100	1	0	-4.861880	-2.032560	2.716461
101	1	0	-3.097585	-2.092127	2.840398
102	1	0	-3.940377	-0.544261	3.016594
103	6	0	-3.632926	-2.642242	0.273129
104	1	0	-2.749207	-3.144629	0.666837
105	1	0	-4.498849	-3.288014	0.451509
106	1	0	-3.504670	-2.521634	-0.804706
107	6	0	-6.108681	-1.226377	-0.282861
108	1	0	-6.625450	-1.812605	0.485154
109	1	0	-6.835196	-0.539487	-0.727826
110	1	0	-5.764531	-1.904038	-1.066001
111	6	0	-0.291103	-2.431920	1.587278
112	1	0	-0.496964	-1.393425	1.815568
113	1	0	0.431919	-3.977014	-3.455004
114	1	0	0.402702	-5.660783	-1.629852
115	6	0	-0.297569	-3.372276	2.595958
116	1	0	-0.465198	-3.063362	3.624474
117	6	0	0.067718	-5.136776	0.991421
118	1	0	0.197283	-6.188632	0.746782
119	6	0	-0.111725	-4.743260	2.297289
120	1	0	-0.123696	-5.479797	3.095914

IV



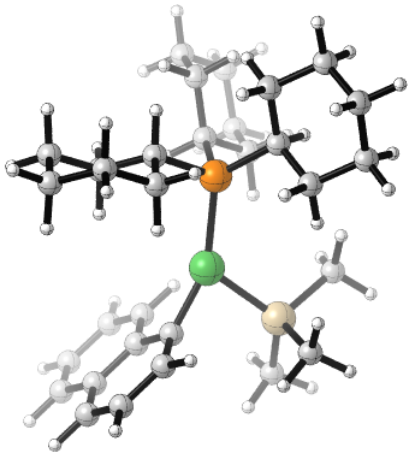
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -4107.097769 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.963145 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.709667	-3.525303	-2.013502
2	6	0	-0.879475	-2.693898	-1.222870
3	6	0	-3.566177	-3.079630	-0.528179
4	6	0	-1.339164	-2.015656	-0.094459
5	6	0	-2.715068	-2.240018	0.273175
6	6	0	-3.033101	-3.712677	-1.682447
7	6	0	-2.337587	1.325987	-1.726438
8	6	0	-3.063528	0.385282	-3.984954
9	6	0	-4.802878	0.978740	-2.249226

10	6	0	-4.445801	0.043882	-3.412192
11	6	0	-3.198660	4.202558	2.682660
12	6	0	-2.502673	2.922623	3.166549
13	6	0	0.435529	2.279424	-1.442494
14	6	0	1.244229	3.759028	-3.354510
15	6	0	2.650595	3.540800	-1.266219
16	6	0	2.248203	4.457326	-2.428421
17	6	0	1.418733	3.018780	-0.508761
18	6	0	0.017049	3.231417	-2.587215
19	6	0	-2.398361	4.869855	1.556447
20	6	0	-3.724062	0.967231	-1.150766
21	6	0	-1.986059	0.367185	-2.887913
22	6	0	-1.449755	2.605695	0.865704
23	6	0	-2.245536	1.939879	2.011564
24	6	0	-2.141172	3.900047	0.388496
25	6	0	-4.923250	-3.264331	-0.141071
26	1	0	-0.540368	4.085684	-2.182500
27	1	0	0.996202	1.448730	-1.890746
28	1	0	0.916583	4.442130	-4.147802
29	1	0	3.314402	4.075171	-0.574419
30	1	0	3.133723	4.774411	-2.992645
31	1	0	1.732841	2.360663	0.303098
32	1	0	-3.098046	1.381109	-4.451722
33	1	0	-4.923027	2.003579	-2.631257
34	1	0	-0.650466	2.733901	-3.294600
35	1	0	-3.688777	-0.022420	-0.688242
36	1	0	-1.889376	-0.648331	-2.492223
37	1	0	-2.409922	2.344326	-2.131097
38	1	0	-2.793170	-0.322422	-4.778233
39	1	0	-5.767692	0.692804	-1.813563
40	1	0	-5.210385	0.102119	-4.196752
41	1	0	-4.010567	1.672119	-0.364723
42	1	0	-1.012510	0.620962	-3.323812
43	1	0	-4.438148	-0.993211	-3.051284
44	1	0	0.159268	-2.580930	-1.525146
45	1	0	-1.434388	5.217186	1.955984
46	1	0	-1.543608	3.189867	3.633803
47	1	0	-4.203273	3.951621	2.313183
48	1	0	-3.205576	1.562932	1.640502
49	1	0	-3.099713	3.657162	-0.086494
50	1	0	-0.483583	2.891917	1.303144
51	1	0	-2.921659	5.761315	1.189319
52	1	0	-3.100861	2.432044	3.943931
53	1	0	-3.338450	4.901171	3.516439
54	1	0	-1.692917	1.068440	2.378110
55	1	0	-1.536090	4.401038	-0.373629
56	1	0	-1.292905	-4.019667	-2.888835
57	1	0	1.740335	2.916117	-3.857589
58	1	0	3.221182	2.685370	-1.650230
59	1	0	1.791568	5.372725	-2.025475
60	1	0	0.911324	3.873897	-0.042480
61	15	0	-0.931557	1.354020	-0.460901
62	28	0	-0.161196	-0.800048	0.714504
63	14	0	0.225620	-2.539641	2.179589
64	5	0	3.522709	-0.740203	-0.071959
65	6	0	-0.186808	-1.880104	3.937334
66	1	0	-1.256768	-1.667675	4.040249
67	1	0	0.076598	-2.622929	4.701943
68	1	0	0.355591	-0.956524	4.165729
69	6	0	2.064380	-3.096851	2.266007

70	1	0	2.405973	-3.514005	1.313144
71	1	0	2.766561	-2.305992	2.543693
72	1	0	2.156791	-3.890806	3.018831
73	6	0	-0.692910	-4.209089	2.064713
74	1	0	-0.498040	-4.714160	1.113225
75	1	0	-0.349120	-4.867245	2.873447
76	1	0	-1.776082	-4.096411	2.159209
77	8	0	3.457009	-0.152794	1.188657
78	6	0	2.469842	0.426918	1.884959
79	8	0	1.279589	0.272739	1.644939
80	6	0	2.995212	1.251763	3.063212
81	6	0	1.835994	2.002035	3.736236
82	1	0	2.218532	2.571878	4.588754
83	1	0	1.359380	2.703410	3.045455
84	1	0	1.069298	1.313787	4.098945
85	6	0	3.648013	0.272607	4.071148
86	1	0	2.921252	-0.451022	4.451879
87	1	0	4.475566	-0.275276	3.613919
88	1	0	4.037862	0.841541	4.921291
89	6	0	4.058680	2.254241	2.560995
90	1	0	3.636867	2.959016	1.837145
91	1	0	4.437367	2.833348	3.408997
92	1	0	4.902156	1.741636	2.093082
93	6	0	4.227474	-2.202728	-1.653924
94	6	0	3.574298	-0.929262	-2.330752
95	8	0	4.392223	-1.768270	-0.269865
96	8	0	2.902417	-0.278774	-1.197424
97	6	0	3.306541	-3.426857	-1.631280
98	1	0	3.175322	-3.846253	-2.632989
99	1	0	3.754137	-4.194278	-0.994286
100	1	0	2.322896	-3.183847	-1.222752
101	6	0	2.534393	-1.228704	-3.405652
102	1	0	2.132530	-0.291771	-3.801813
103	1	0	2.989139	-1.777219	-4.237016
104	1	0	1.701923	-1.813524	-3.013550
105	6	0	4.609165	0.072389	-2.856336
106	1	0	5.130785	-0.319167	-3.734319
107	1	0	4.100946	0.995844	-3.145771
108	1	0	5.353628	0.317747	-2.093567
109	6	0	5.602270	-2.589472	-2.194929
110	1	0	5.980639	-3.450996	-1.638200
111	1	0	5.539065	-2.871059	-3.251042
112	1	0	6.324308	-1.777928	-2.090978
113	1	0	-3.676452	-4.352467	-2.281595
114	1	0	-5.555857	-3.898416	-0.758638
115	6	0	-3.281867	-1.651195	1.438406
116	1	0	-2.637309	-1.029183	2.050743
117	6	0	-4.597640	-1.854887	1.794767
118	1	0	-4.996900	-1.395467	2.695153
119	6	0	-5.432067	-2.668162	0.990475
120	1	0	-6.469824	-2.825515	1.272156

V

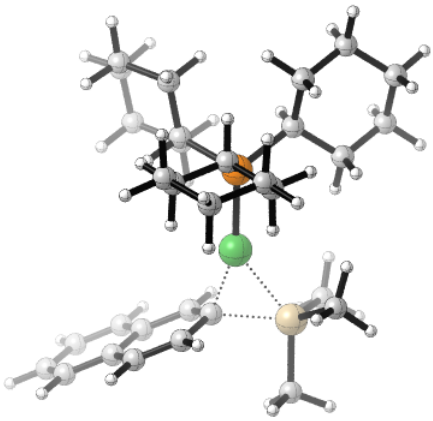


E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3349.522294 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.662105 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.743923	0.321962	0.585966
2	6	0	-3.486318	0.205299	-0.100814
3	6	0	-4.169113	-1.598846	1.955088
4	6	0	-2.549980	-0.828016	0.271861
5	6	0	-2.929490	-1.714450	1.277760
6	6	0	-5.057790	-0.603515	1.617838
7	6	0	1.427983	0.908098	1.886226
8	6	0	0.378818	2.519537	3.565787
9	6	0	1.272674	0.292630	4.360809
10	6	0	0.216279	1.382375	4.583299
11	6	0	5.143231	-2.696480	0.488898
12	6	0	3.888554	-3.144680	-0.273622
13	6	0	1.593970	1.770699	-0.952795
14	6	0	2.786025	3.936706	-1.544117
15	6	0	1.475204	2.695750	-3.321449
16	6	0	2.678785	3.606351	-3.039558
17	6	0	1.499598	1.425371	-2.454806
18	6	0	2.826087	2.659836	-0.685508
19	6	0	5.399469	-1.194743	0.301124
20	6	0	1.247012	-0.231949	2.915488
21	6	0	0.358250	2.000458	2.117395
22	6	0	2.921075	-0.794126	-0.112506
23	6	0	2.658931	-2.302073	0.104245
24	6	0	4.168038	-0.355445	0.687337
25	1	0	3.739128	2.102678	-0.931369
26	1	0	0.698079	2.361060	-0.711711
27	1	0	3.679273	4.542267	-1.348860
28	1	0	1.445715	2.419173	-4.382068
29	1	0	2.606074	4.527981	-3.628952
30	1	0	0.605383	0.824215	-2.644180
31	1	0	1.331694	3.037021	3.748690
32	1	0	2.269697	0.700567	4.581597
33	1	0	2.896232	2.929597	0.374366
34	1	0	0.287065	-0.733223	2.728458
35	1	0	-0.637310	1.589126	1.895592
36	1	0	2.417004	1.359261	2.042355
37	1	0	-0.412043	3.267380	3.697144

38	1	0	1.116293	-0.540514	5.056349
39	1	0	0.280351	1.774219	5.605312
40	1	0	2.022760	-0.994392	2.789460
41	1	0	0.507357	2.841022	1.431542
42	1	0	-0.785041	0.942394	4.477415
43	1	0	-2.261455	-2.523670	1.562827
44	1	0	5.655046	-0.997457	-0.749768
45	1	0	4.068132	-3.052337	-1.354346
46	1	0	5.010418	-2.908010	1.559585
47	1	0	2.407972	-2.484034	1.157740
48	1	0	3.976657	-0.485825	1.759855
49	1	0	3.143816	-0.656743	-1.181242
50	1	0	6.264023	-0.876604	0.896275
51	1	0	3.683375	-4.204722	-0.082935
52	1	0	6.015692	-3.275095	0.163095
53	1	0	1.789449	-2.620090	-0.476509
54	1	0	4.382792	0.706100	0.536759
55	1	0	1.923048	4.547273	-1.242773
56	1	0	0.547288	3.248769	-3.117720
57	1	0	3.599732	3.100509	-3.363684
58	1	0	2.360492	0.808495	-2.748821
59	15	0	1.353787	0.238431	0.123616
60	28	0	-0.752623	-0.616885	-0.109794
61	14	0	-1.206570	-2.156996	-1.675541
62	6	0	-1.105637	-3.901304	-0.902609
63	1	0	-1.949230	-4.081242	-0.229495
64	1	0	-1.143278	-4.659874	-1.695327
65	1	0	-0.183481	-4.060201	-0.333771
66	6	0	0.161385	-2.078329	-3.021446
67	1	0	0.044790	-1.193508	-3.656119
68	1	0	1.176232	-2.064672	-2.612966
69	1	0	0.074322	-2.960514	-3.670104
70	6	0	-2.830080	-2.103982	-2.670616
71	1	0	-3.691914	-2.342105	-2.040472
72	1	0	-3.010505	-1.119435	-3.113820
73	1	0	-2.790239	-2.836040	-3.487400
74	6	0	-3.207217	1.142398	-1.135612
75	6	0	-5.644021	1.359153	0.217378
76	6	0	-5.332454	2.249642	-0.785192
77	1	0	-6.032389	3.035672	-1.055218
78	6	0	-4.099395	2.138313	-1.471185
79	1	0	-3.861269	2.837226	-2.268504
80	1	0	-6.591695	1.436437	0.745746
81	1	0	-6.012258	-0.513548	2.131110
82	1	0	-4.416948	-2.306419	2.742923
83	1	0	-2.263382	1.046253	-1.666487

$TS_{V\text{-}VI}$



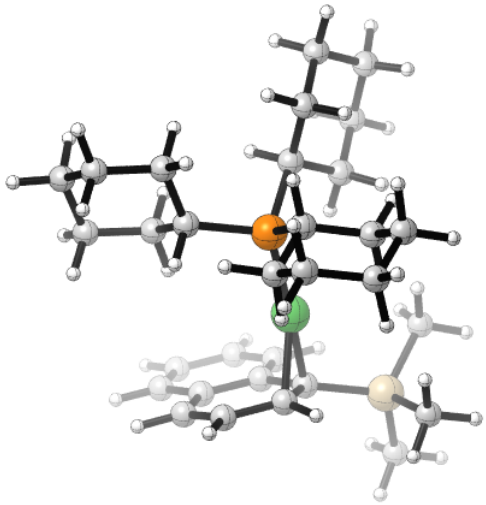
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3349.522322 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.662597 Hartrees
Imaginary Frequency: -129.1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.515625	-1.165318	-0.935430
2	6	0	-3.296088	-2.016525	-3.211103
3	6	0	-3.053667	-3.639301	-1.286695
4	6	0	-2.962961	-3.459255	-2.807974
5	6	0	-2.829041	-1.004525	4.437606
6	6	0	-1.367998	-0.619677	4.163903
7	6	0	-1.905199	1.737472	-0.677508
8	6	0	-3.676501	3.467805	-1.255254
9	6	0	-1.313235	4.213922	-0.724664
10	6	0	-2.802621	4.581195	-0.660309
11	6	0	-1.030046	2.853503	-0.065162
12	6	0	-3.398522	2.110469	-0.583677
13	6	0	-3.788168	-0.210751	3.539432
14	6	0	-2.171983	-2.620343	-0.545841
15	6	0	-2.417629	-0.995508	-2.467329
16	6	0	-1.970785	0.044086	1.775670
17	6	0	-1.011174	-0.765481	2.675837
18	6	0	-3.434140	-0.366164	2.048953
19	1	0	-3.695232	2.174162	0.471577
20	1	0	-1.636859	1.679402	-1.741636
21	1	0	-4.739143	3.721493	-1.156822
22	1	0	-0.706941	4.991466	-0.244782
23	1	0	-2.986043	5.528226	-1.182051
24	1	0	0.029622	2.595899	-0.167771
25	1	0	-4.353274	-1.813372	-2.987223
26	1	0	-4.098965	-3.516306	-0.968447
27	1	0	-4.026284	1.336747	-1.040894
28	1	0	-1.115820	-2.804488	-0.785601
29	1	0	-1.369808	-1.121552	-2.773099
30	1	0	-3.551781	-0.960417	-0.634933
31	1	0	-3.177478	-1.884963	-4.293520
32	1	0	-2.760093	-4.657304	-1.003301
33	1	0	-3.633189	-4.161984	-3.317400
34	1	0	-2.270241	-2.764838	0.535705
35	1	0	-2.710477	0.016944	-2.765105
36	1	0	-1.943564	-3.701749	-3.140177
37	1	0	-3.742895	0.853442	3.811748

38	1	0	-1.205068	0.423288	4.471418
39	1	0	-2.962078	-2.079107	4.246486
40	1	0	-1.053945	-1.827311	2.396083
41	1	0	-3.583234	-1.414842	1.761182
42	1	0	-1.864357	1.099363	2.066728
43	1	0	-4.823544	-0.530960	3.708724
44	1	0	-0.690710	-1.232299	4.770911
45	1	0	-3.075750	-0.843290	5.493837
46	1	0	0.021488	-0.443188	2.499566
47	1	0	-4.127901	0.224023	1.442091
48	1	0	-3.474312	3.383705	-2.332639
49	1	0	-0.994357	4.174440	-1.775900
50	1	0	-3.090500	4.742682	0.388674
51	1	0	-1.232268	2.934624	1.012620
52	15	0	-1.383993	0.041568	-0.029763
53	28	0	0.755449	-0.299446	-0.320238
54	6	0	2.719441	-0.491046	-0.537094
55	6	0	3.200768	0.799688	-0.033111
56	6	0	2.071672	-0.480044	-1.819005
57	6	0	3.125858	1.976069	-0.854593
58	6	0	2.029704	0.710415	-2.624704
59	1	0	1.865100	-1.420349	-2.325151
60	6	0	2.550297	1.887385	-2.166801
61	1	0	1.589767	0.655492	-3.617826
62	14	0	3.315454	-2.154725	0.165746
63	6	0	5.214464	-2.200740	0.176587
64	1	0	5.610103	-2.096202	-0.839793
65	1	0	5.642292	-1.392988	0.778552
66	1	0	5.581426	-3.151370	0.581237
67	6	0	2.706850	-3.564394	-0.947285
68	1	0	3.051832	-4.524805	-0.546751
69	1	0	1.613319	-3.599947	-0.997696
70	1	0	3.090371	-3.479198	-1.969525
71	6	0	2.687888	-2.526733	1.920446
72	1	0	3.014828	-1.795038	2.665705
73	1	0	1.593594	-2.556025	1.944569
74	1	0	3.055812	-3.508575	2.242473
75	1	0	2.526314	2.782717	-2.783406
76	6	0	3.616846	3.206029	-0.360567
77	1	0	3.552537	4.083417	-1.000291
78	6	0	4.167767	3.306586	0.904215
79	1	0	4.538720	4.260869	1.266973
80	6	0	4.243791	2.161800	1.717824
81	1	0	4.672610	2.231558	2.713808
82	6	0	3.775775	0.942891	1.255601
83	1	0	3.842894	0.074574	1.901948

VI



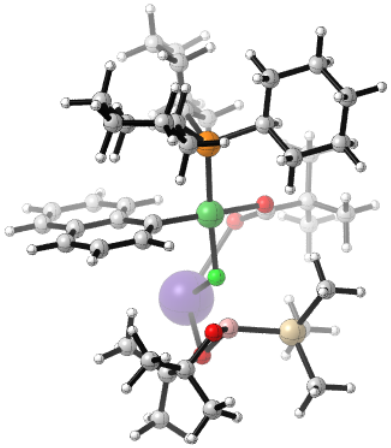
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3349.545150 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.661939 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.743923	0.321962	0.585966
2	6	0	-3.486318	0.205299	-0.100814
3	6	0	-4.169113	-1.598846	1.955088
4	6	0	-2.549980	-0.828016	0.271861
5	6	0	-2.929490	-1.714450	1.277760
6	6	0	-5.057790	-0.603515	1.617838
7	6	0	1.427983	0.908098	1.886226
8	6	0	0.378818	2.519537	3.565787
9	6	0	1.272674	0.292630	4.360809
10	6	0	0.216279	1.382375	4.583299
11	6	0	5.143231	-2.696480	0.488898
12	6	0	3.888554	-3.144680	-0.273622
13	6	0	1.593970	1.770699	-0.952795
14	6	0	2.786025	3.936706	-1.544117
15	6	0	1.475204	2.695750	-3.321449
16	6	0	2.678785	3.606351	-3.039558
17	6	0	1.499598	1.425371	-2.454806
18	6	0	2.826087	2.659836	-0.685508
19	6	0	5.399469	-1.194743	0.301124
20	6	0	1.247012	-0.231949	2.915488
21	6	0	0.358250	2.000458	2.117395
22	6	0	2.921075	-0.794126	-0.112506
23	6	0	2.658931	-2.302073	0.104245
24	6	0	4.168038	-0.355445	0.687337
25	1	0	3.739128	2.102678	-0.931369
26	1	0	0.698079	2.361060	-0.711711
27	1	0	3.679273	4.542267	-1.348860
28	1	0	1.445715	2.419173	-4.382068
29	1	0	2.606074	4.527981	-3.628952
30	1	0	0.605383	0.824215	-2.644180
31	1	0	1.331694	3.037021	3.748690
32	1	0	2.269697	0.700567	4.581597
33	1	0	2.896232	2.929597	0.374366
34	1	0	0.287065	-0.733223	2.728458
35	1	0	-0.637310	1.589126	1.895592

36	1	0	2.417004	1.359261	2.042355
37	1	0	-0.412043	3.267380	3.697144
38	1	0	1.116293	-0.540514	5.056349
39	1	0	0.280351	1.774219	5.605312
40	1	0	2.022760	-0.994392	2.789460
41	1	0	0.507357	2.841022	1.431542
42	1	0	-0.785041	0.942394	4.477415
43	1	0	-2.261455	-2.523670	1.562827
44	1	0	5.655046	-0.997457	-0.749768
45	1	0	4.068132	-3.052337	-1.354346
46	1	0	5.010418	-2.908010	1.559585
47	1	0	2.407972	-2.484034	1.157740
48	1	0	3.976657	-0.485825	1.759855
49	1	0	3.143816	-0.656743	-1.181242
50	1	0	6.264023	-0.876604	0.896275
51	1	0	3.683375	-4.204722	-0.082935
52	1	0	6.015692	-3.275095	0.163095
53	1	0	1.789449	-2.620090	-0.476509
54	1	0	4.382792	0.706100	0.536759
55	1	0	1.923048	4.547273	-1.242773
56	1	0	0.547288	3.248769	-3.117720
57	1	0	3.599732	3.100509	-3.363684
58	1	0	2.360492	0.808495	-2.748821
59	15	0	1.353787	0.238431	0.123616
60	28	0	-0.752623	-0.616885	-0.109794
61	14	0	-1.206570	-2.156996	-1.675541
62	6	0	-1.105637	-3.901304	-0.902609
63	1	0	-1.949230	-4.081242	-0.229495
64	1	0	-1.143278	-4.659874	-1.695327
65	1	0	-0.183481	-4.060201	-0.333771
66	6	0	0.161385	-2.078329	-3.021446
67	1	0	0.044790	-1.193508	-3.656119
68	1	0	1.176232	-2.064672	-2.612966
69	1	0	0.074322	-2.960514	-3.670104
70	6	0	-2.830080	-2.103982	-2.670616
71	1	0	-3.691914	-2.342105	-2.040472
72	1	0	-3.010505	-1.119435	-3.113820
73	1	0	-2.790239	-2.836040	-3.487400
74	6	0	-3.207217	1.142398	-1.135612
75	6	0	-5.644021	1.359153	0.217378
76	6	0	-5.332454	2.249642	-0.785192
77	1	0	-6.032389	3.035672	-1.055218
78	6	0	-4.099395	2.138313	-1.471185
79	1	0	-3.861269	2.837226	-2.268504
80	1	0	-6.591695	1.436437	0.745746
81	1	0	-6.012258	-0.513548	2.131110
82	1	0	-4.416948	-2.306419	2.742923
83	1	0	-2.263382	1.046253	-1.666487

CsF pathway

III-Cs



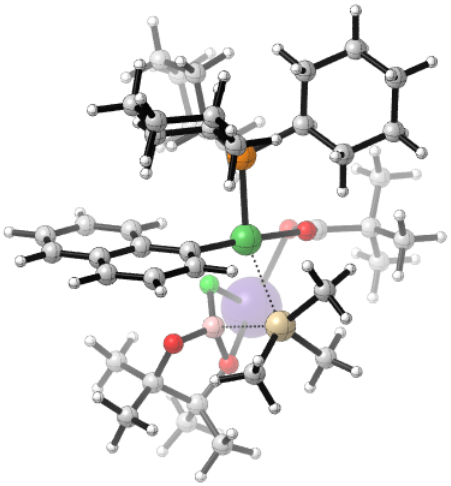
E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -4227.180441 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.961408 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.133004	-3.867475	1.301889
2	6	0	0.109181	-2.451856	1.187238
3	6	0	-0.457799	-3.986907	-1.094486
4	6	0	0.081172	-1.808047	-0.099007
5	6	0	-0.235872	-2.590010	-1.199062
6	6	0	-0.396671	-4.619676	0.127422
7	6	0	3.340892	-1.582194	-1.405123
8	6	0	4.086600	-4.012681	-1.395029
9	6	0	3.584560	-2.869442	-3.591009
10	6	0	3.563096	-4.198480	-2.824838
11	6	0	4.161943	3.173103	-3.608816
12	6	0	2.702474	3.198003	-3.136165
13	6	0	3.444505	-0.206856	1.184724
14	6	0	5.499769	-0.675586	2.602517
15	6	0	3.613444	0.722662	3.543159
16	6	0	5.125053	0.460362	3.563693
17	6	0	3.084641	0.965374	2.118409
18	6	0	4.977899	-0.404040	1.179857
19	6	0	5.095742	2.702966	-2.486084
20	6	0	2.816282	-1.762460	-2.846880
21	6	0	3.298721	-2.926502	-0.641843
22	6	0	3.196147	1.402717	-1.402572
23	6	0	2.261272	1.843556	-2.555674
24	6	0	4.654996	1.344453	-1.909979
25	1	0	5.461077	0.505571	0.803540
26	1	0	2.995404	-1.110701	1.619414
27	1	0	6.587783	-0.811729	2.575401
28	1	0	3.366323	1.582709	4.177424
29	1	0	5.460851	0.226646	4.581207
30	1	0	2.004859	1.121625	2.154543
31	1	0	5.151201	-3.737827	-1.431022
32	1	0	4.627969	-2.552076	-3.733644
33	1	0	5.281422	-1.220533	0.518702
34	1	0	1.751965	-2.013124	-2.815832
35	1	0	2.263066	-3.252470	-0.525848

36	1	0	4.397755	-1.291599	-1.483351
37	1	0	4.026669	-4.956421	-0.839979
38	1	0	3.159696	-2.997126	-4.593961
39	1	0	4.155984	-4.953311	-3.355486
40	1	0	2.903762	-0.829158	-3.409499
41	1	0	3.709834	-2.818984	0.366323
42	1	0	2.532842	-4.577649	-2.783333
43	1	0	-0.337902	-2.125969	-2.175589
44	1	0	5.101291	3.450471	-1.679975
45	1	0	2.584645	3.972608	-2.365603
46	1	0	4.255134	2.489659	-4.465197
47	1	0	2.278852	1.096216	-3.358613
48	1	0	4.738956	0.587398	-2.700414
49	1	0	3.127019	2.180798	-0.631497
50	1	0	6.128035	2.629369	-2.849779
51	1	0	2.036408	3.477358	-3.960863
52	1	0	4.467006	4.163772	-3.966949
53	1	0	1.233651	1.913361	-2.199008
54	1	0	5.345139	1.044886	-1.117474
55	1	0	5.075224	-1.621188	2.968728
56	1	0	3.089502	-0.143106	3.972949
57	1	0	5.655086	1.375190	3.261965
58	1	0	3.525857	1.890127	1.724922
59	15	0	2.557071	-0.126126	-0.486671
60	28	0	0.317084	0.074303	-0.208797
61	14	0	-3.347631	2.282700	-1.614737
62	5	0	-3.167540	0.291541	-1.162692
63	6	0	-1.896358	2.952931	-2.643717
64	1	0	-1.828877	2.403211	-3.590100
65	1	0	-2.008438	4.017154	-2.883896
66	1	0	-0.952660	2.818017	-2.108700
67	6	0	-3.543211	3.330394	-0.019300
68	1	0	-4.455867	3.030654	0.513324
69	1	0	-2.691832	3.207063	0.658375
70	1	0	-3.635098	4.401124	-0.237243
71	6	0	-4.933161	2.647442	-2.618745
72	1	0	-4.926138	2.134772	-3.586567
73	1	0	-5.837350	2.333850	-2.083697
74	1	0	-5.026400	3.722466	-2.817074
75	8	0	-0.260190	1.936604	2.098257
76	6	0	0.167666	2.577169	1.110570
77	8	0	0.511799	2.043598	-0.008209
78	6	0	0.380125	4.115600	1.245052
79	6	0	1.858211	4.349612	1.634157
80	1	0	2.043622	5.421650	1.767600
81	1	0	2.108401	3.845005	2.572810
82	1	0	2.535277	3.987082	0.854768
83	6	0	0.091000	4.844475	-0.077559
84	1	0	0.710204	4.451424	-0.886041
85	1	0	-0.954392	4.734065	-0.376185
86	1	0	0.299628	5.915408	0.031587
87	6	0	-0.516116	4.678994	2.362935
88	1	0	-0.333534	4.162147	3.307861
89	1	0	-0.314923	5.747361	2.502577
90	1	0	-1.576986	4.571162	2.115418
91	6	0	-4.561661	-1.520645	-0.590470
92	6	0	-4.196539	-1.565848	-2.125006
93	8	0	-4.144289	-0.191323	-0.210022
94	8	0	-3.091739	-0.655072	-2.221417
95	6	0	0.349903	-1.725040	2.392811

96	6	0	-0.109644	-4.476963	2.587663
97	6	0	0.128078	-3.739763	3.725694
98	1	0	0.144238	-4.223883	4.698363
99	6	0	0.356634	-2.344764	3.626238
100	1	0	0.552349	-1.765018	4.525325
101	1	0	-0.288691	-5.547760	2.656328
102	1	0	-0.562940	-5.690891	0.211045
103	1	0	-0.681995	-4.559772	-1.991382
104	1	0	0.520104	-0.653033	2.324528
105	9	0	-1.664592	0.238876	-0.332786
106	55	0	-2.720300	0.387561	2.454936
107	6	0	-3.774476	-2.546463	0.240415
108	1	0	-3.986054	-2.389617	1.306154
109	1	0	-4.069134	-3.574599	0.008629
110	1	0	-2.700774	-2.448354	0.075585
111	6	0	-6.055381	-1.658996	-0.280141
112	1	0	-6.442627	-2.626627	-0.618088
113	1	0	-6.217203	-1.598113	0.802330
114	1	0	-6.638957	-0.865793	-0.750161
115	6	0	-5.329604	-1.037037	-3.023610
116	1	0	-4.935087	-0.903631	-4.035097
117	1	0	-6.173476	-1.733472	-3.073958
118	1	0	-5.697207	-0.068951	-2.677860
119	6	0	-3.760164	-2.939503	-2.639485
120	1	0	-4.569388	-3.672400	-2.541111
121	1	0	-3.503594	-2.863584	-3.700792
122	1	0	-2.885367	-3.308700	-2.105004

$TS_{III\text{-}IV}$-Cs



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -4227.151860 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.962375 Hartrees
Imaginary Frequency: -95.0

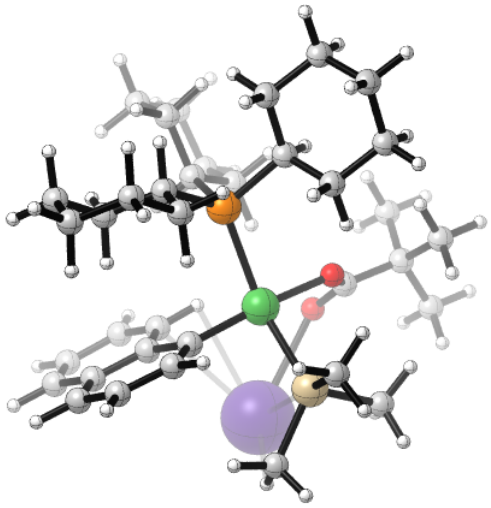
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230183	4.247813	0.379274
2	6	0	-0.170613	2.812112	0.484585
3	6	0	-0.783794	4.051036	-1.964845
4	6	0	-0.411987	1.982213	-0.671973
5	6	0	-0.725792	2.639091	-1.854753
6	6	0	-0.538194	4.846107	-0.870900

7	6	0	-3.837312	1.255257	-0.127461
8	6	0	-4.789263	3.539949	0.435654
9	6	0	-5.298390	2.495276	-1.806934
10	6	0	-5.082218	3.810090	-1.046068
11	6	0	-5.262821	-3.439813	-1.982900
12	6	0	-3.763228	-3.358610	-2.291218
13	6	0	-2.468122	-0.178570	2.053738
14	6	0	-3.531146	-0.052195	4.353299
15	6	0	-1.284666	-1.183527	4.063451
16	6	0	-2.587255	-1.144528	4.874977
17	6	0	-1.544286	-1.308626	2.551737
18	6	0	-3.794796	-0.208783	2.844007
19	6	0	-5.527980	-3.114162	-0.508240
20	6	0	-4.120250	1.521750	-1.622058
21	6	0	-3.589333	2.591881	0.604881
22	6	0	-3.424041	-1.671388	-0.402800
23	6	0	-3.157608	-2.001967	-1.889129
24	6	0	-4.943773	-1.743433	-0.120289
25	1	0	-4.299821	-1.169103	2.683230
26	1	0	-1.969076	0.769753	2.292103
27	1	0	-4.482575	-0.077651	4.898994
28	1	0	-0.652499	-2.016313	4.397327
29	1	0	-2.373566	-0.988194	5.939621
30	1	0	-0.595231	-1.319618	2.010407
31	1	0	-5.679601	3.100452	0.910017
32	1	0	-6.221649	2.018007	-1.446322
33	1	0	-4.484304	0.573176	2.511079
34	1	0	-3.220493	1.940380	-2.083649
35	1	0	-2.699252	3.074157	0.199005
36	1	0	-4.749080	0.821637	0.303980
37	1	0	-4.586552	4.480190	0.962263
38	1	0	-5.447502	2.690280	-2.876101
39	1	0	-5.958518	4.461272	-1.153410
40	1	0	-4.344109	0.590710	-2.149779
41	1	0	-3.399338	2.430760	1.670310
42	1	0	-4.230722	4.347390	-1.485258
43	1	0	-0.925712	2.064243	-2.753622
44	1	0	-5.078297	-3.893509	0.123767
45	1	0	-3.246141	-4.162271	-1.748958
46	1	0	-5.806095	-2.722442	-2.614719
47	1	0	-3.593955	-1.225397	-2.528870
48	1	0	-5.461806	-0.973908	-0.706373
49	1	0	-2.928191	-2.450496	0.192970
50	1	0	-6.604690	-3.125523	-0.298083
51	1	0	-3.580208	-3.539163	-3.357633
52	1	0	-5.653551	-4.433937	-2.232203
53	1	0	-2.083924	-1.998638	-2.071263
54	1	0	-5.167879	-1.538088	0.928643
55	1	0	-3.088987	0.936138	4.542318
56	1	0	-0.715594	-0.261513	4.252057
57	1	0	-3.089461	-2.119672	4.796853
58	1	0	-2.015428	-2.282032	2.353668
59	15	0	-2.529466	-0.088114	0.162949
60	28	0	-0.307263	0.067311	-0.647204
61	14	0	1.434874	0.052582	-2.592836
62	5	0	2.510657	0.696362	-0.411886
63	6	0	-0.100644	-0.538284	-3.607167
64	1	0	-0.989549	0.092058	-3.512033
65	1	0	0.200424	-0.525645	-4.664100
66	1	0	-0.376310	-1.559770	-3.342866

67	6	0	2.653086	-1.384565	-2.988532
68	1	0	3.688385	-1.125972	-2.758819
69	1	0	2.390377	-2.273650	-2.404558
70	1	0	2.584562	-1.656773	-4.049516
71	6	0	1.983486	1.585209	-3.621329
72	1	0	2.340572	2.404516	-2.995543
73	1	0	2.770260	1.310422	-4.335019
74	1	0	1.140958	1.965562	-4.207818
75	8	0	0.933261	-2.746474	1.029783
76	6	0	0.394448	-2.865270	-0.092752
77	8	0	-0.157295	-1.932389	-0.774703
78	6	0	0.362926	-4.309484	-0.694813
79	6	0	-0.662704	-5.118641	0.130214
80	1	0	-0.685871	-6.163808	-0.200414
81	1	0	-0.405767	-5.094015	1.193200
82	1	0	-1.672576	-4.710775	0.015906
83	6	0	-0.011668	-4.344056	-2.182559
84	1	0	-0.997176	-3.912876	-2.358102
85	1	0	0.706739	-3.787167	-2.789907
86	1	0	-0.026566	-5.380335	-2.541973
87	6	0	1.755249	-4.950295	-0.512368
88	1	0	2.038376	-4.954997	0.544026
89	1	0	1.752086	-5.985625	-0.871461
90	1	0	2.518603	-4.408417	-1.085340
91	6	0	4.803104	1.181644	-0.677793
92	6	0	3.992438	2.453384	-0.194673
93	8	0	3.831096	0.120145	-0.546592
94	8	0	2.634565	2.095295	-0.490408
95	6	0	0.120400	2.271260	1.769121
96	6	0	0.003591	5.048108	1.531938
97	6	0	0.274733	4.479922	2.755706
98	1	0	0.444713	5.106771	3.627267
99	6	0	0.330678	3.070809	2.872857
100	1	0	0.548345	2.618617	3.837581
101	1	0	-0.042955	6.130123	1.426765
102	1	0	-0.580918	5.930434	-0.943057
103	1	0	-1.022632	4.500822	-2.926228
104	1	0	0.207564	1.196676	1.861272
105	9	0	1.879058	0.138437	0.719026
106	55	0	3.671059	-2.102045	1.540219
107	6	0	6.013203	0.829810	0.199402
108	1	0	5.735742	0.682166	1.246906
109	1	0	6.483734	-0.087470	-0.173167
110	1	0	6.768416	1.621937	0.165877
111	6	0	4.084553	2.694087	1.324288
112	1	0	5.077958	3.039634	1.630842
113	1	0	3.349565	3.454299	1.599116
114	1	0	3.835288	1.788813	1.885470
115	6	0	4.328313	3.752220	-0.928784
116	1	0	3.677792	4.550565	-0.560908
117	1	0	5.367952	4.050080	-0.751833
118	1	0	4.168798	3.660516	-2.004169
119	6	0	5.273757	1.259796	-2.136256
120	1	0	6.059400	2.011657	-2.261756
121	1	0	5.684057	0.289429	-2.433516
122	1	0	4.453112	1.498358	-2.811008

IV-Cs



E at M06/def2tzvpp (SDD, Ni) (IEFPCM, Toluene) = -3716.105675 Hartrees
Correction to Free Gibbs Energy (B3LYP/6-31G**(SDD,Ni)) = 0.785686 Hartrees
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.445063	3.852120	0.321808
2	6	0	1.169003	2.436970	0.300912
3	6	0	0.722858	4.002192	-1.976812
4	6	0	0.689753	1.773499	-0.896724
5	6	0	0.478292	2.607825	-1.994935
6	6	0	1.209815	4.621504	-0.846844
7	6	0	-2.981931	1.559398	-0.279705
8	6	0	-3.438032	4.045717	0.032437
9	6	0	-4.038047	2.933189	-2.155337
10	6	0	-3.571886	4.232227	-1.484517
11	6	0	-4.888344	-3.102286	-1.925566
12	6	0	-3.370317	-3.253929	-2.088874
13	6	0	-1.917554	0.082046	2.037228
14	6	0	-3.084273	0.403232	4.274951
15	6	0	-0.943368	-0.942664	4.154533
16	6	0	-2.280188	-0.753726	4.884418
17	6	0	-1.129752	-1.102465	2.635272
18	6	0	-3.275999	0.216906	2.758667
19	6	0	-5.237008	-2.567769	-0.530307
20	6	0	-3.118835	1.749649	-1.806946
21	6	0	-2.505270	2.872569	0.380973
22	6	0	-2.964980	-1.422685	-0.359073
23	6	0	-2.614822	-1.951312	-1.771331
24	6	0	-4.495477	-1.253491	-0.229808
25	1	0	-3.869065	-0.691788	2.595681
26	1	0	-1.336902	0.989643	2.256824
27	1	0	-4.061833	0.489359	4.765548
28	1	0	-0.409793	-1.813655	4.554541
29	1	0	-2.112542	-0.581184	5.954706
30	1	0	-0.152973	-1.207322	2.156389
31	1	0	-4.433157	3.861608	0.464029
32	1	0	-5.063373	2.705353	-1.828549
33	1	0	-3.859520	1.051386	2.356420
34	1	0	-2.124921	1.920838	-2.233205
35	1	0	-1.491301	3.105881	0.044131
36	1	0	-3.981791	1.339080	0.118342

37	1	0	-3.061149	4.964263	0.498510
38	1	0	-4.080422	3.058057	-3.244486
39	1	0	-4.268105	5.049540	-1.710074
40	1	0	-3.508491	0.840316	-2.275609
41	1	0	-2.459045	2.764686	1.469720
42	1	0	-2.596316	4.523780	-1.896777
43	1	0	0.119963	2.178032	-2.926875
44	1	0	-4.965621	-3.318781	0.225762
45	1	0	-3.016059	-4.047110	-1.414971
46	1	0	-5.267613	-2.401789	-2.683681
47	1	0	-2.877112	-1.196171	-2.524216
48	1	0	-4.840018	-0.493192	-0.942373
49	1	0	-2.648191	-2.196843	0.354624
50	1	0	-6.319118	-2.410961	-0.438451
51	1	0	-3.125964	-3.582790	-3.106456
52	1	0	-5.392118	-4.059929	-2.105973
53	1	0	-1.539127	-2.119301	-1.842644
54	1	0	-4.774591	-0.894941	0.763985
55	1	0	-2.557732	1.350516	4.458993
56	1	0	-0.302661	-0.069062	4.344580
57	1	0	-2.867913	-1.679823	4.806219
58	1	0	-1.674936	-2.036939	2.442536
59	15	0	-1.892608	0.068756	0.139397
60	28	0	0.376213	-0.102474	-0.813998
61	14	0	1.882465	-0.386348	-2.532920
62	6	0	0.807659	-0.506731	-4.117865
63	1	0	0.254986	0.417247	-4.317329
64	1	0	1.427003	-0.721098	-4.998978
65	1	0	0.074091	-1.314011	-4.017602
66	6	0	2.869598	-2.043685	-2.554261
67	1	0	3.547291	-2.179641	-1.701805
68	1	0	2.182540	-2.894365	-2.541842
69	1	0	3.476471	-2.112981	-3.466545
70	6	0	3.254417	0.895213	-2.996019
71	1	0	2.858130	1.909901	-3.083471
72	1	0	4.090195	0.942644	-2.282517
73	1	0	3.695845	0.617120	-3.961807
74	8	0	1.929049	-2.018968	1.055783
75	6	0	1.128360	-2.623618	0.300704
76	8	0	0.336379	-2.061710	-0.534140
77	6	0	1.066289	-4.174733	0.407242
78	6	0	0.455226	-4.522798	1.782653
79	1	0	0.452738	-5.608342	1.936026
80	1	0	1.030583	-4.059126	2.588857
81	1	0	-0.579923	-4.172730	1.856773
82	6	0	0.219590	-4.802568	-0.709109
83	1	0	-0.805187	-4.425626	-0.687883
84	1	0	0.630513	-4.579736	-1.698213
85	1	0	0.188906	-5.892562	-0.592081
86	6	0	2.504581	-4.730323	0.348116
87	1	0	3.118907	-4.283080	1.133846
88	1	0	2.499245	-5.817705	0.485944
89	1	0	2.972170	-4.517640	-0.619299
90	6	0	1.362471	1.722337	1.521317
91	6	0	1.932149	4.452184	1.517492
92	6	0	2.126981	3.717505	2.665911
93	1	0	2.487675	4.199212	3.570914
94	6	0	1.829722	2.332368	2.669991
95	1	0	1.943285	1.756889	3.586278
96	1	0	2.139446	5.520301	1.511062

97	1	0	1.411290	5.689721	-0.831433
98	1	0	0.532626	4.586211	-2.875070
99	1	0	1.121909	0.660799	1.532002
100	55	0	4.019119	-0.068057	0.588766
