APPENDIX IV: Computational studies

Computational results: Chapter 2

- **Computational methods**

Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the M06-2X hybrid functional,[2] that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, B, N and O. The LANL2DZ basis set was used for Fe. Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Gibbs free energy has been used throughout the schemes. Scan of the potential energy surface was used as implemented in Gaussian by elongation of the critical bond being involved in every elementary step studied. Transition state structure search was performed around the maximum energy regions computed, but no one could be located (except for methyl rotation and skeletal vibrations). The approximate activation energy for the only step that seems to proceed with a barrier was determined from electronic energy computed at intermediate steps of the *scan* calculation, as well as the energy corresponding to the starting alkenyl-Fe complex containing coordinated C-C double bond.

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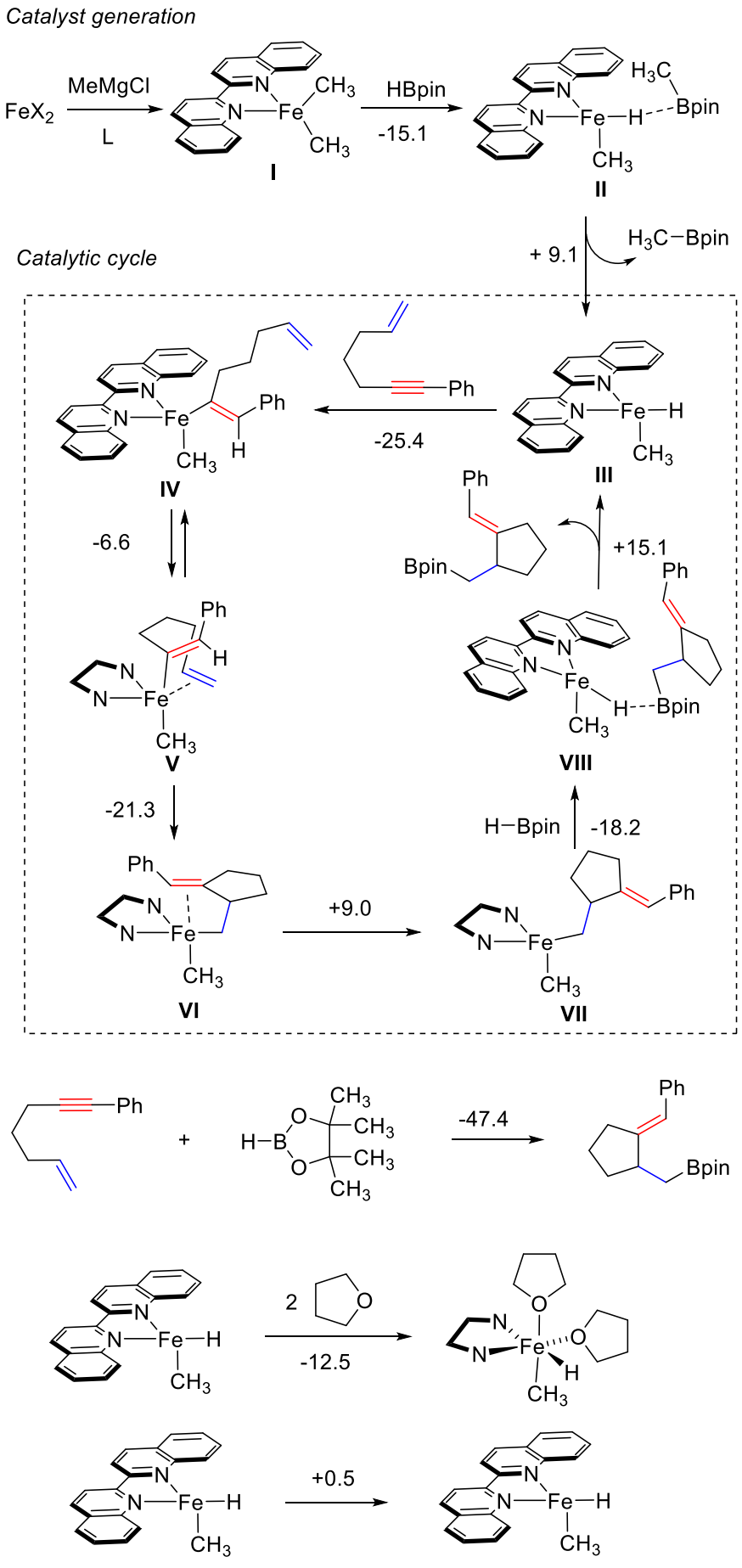
[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. 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, D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

[2] Y. Zhao, D. G. Truhlar, "The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new functionals and systematic testing of four M06-class functionals and 12 other functionals". *Theor Chem Account*. **2008**, *120*, 215–241.


Catalyst generation
FeX2
MeMgCl
L
CH3
HBpin
-15.1
H3C
Bpin
I
II
+ 9.1
H3C–Bpin
Catalytic cycle
Ph
-25.4
III
IV
-6.6
+15.1
V
VIII
-21.3
H–Bpin
-18.2
+9.0
VI
VII
-47.4
2
-12.5
+0.5

- ***Atomic coordinates and energies for the stationary points***

HBpin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.779739	-0.185909	-0.054398
2	6	0	0.779862	-0.185511	0.054641
3	8	0	1.062061	1.183712	0.420802
4	5	0	-0.000428	1.932940	-0.000133
5	8	0	-1.062474	1.183129	-0.421083
6	1	0	-0.000591	3.119857	-0.000450
7	6	0	-1.346529	-1.109755	-1.120035
8	1	0	-1.078366	-2.150475	-0.908074
9	1	0	-0.978688	-0.845474	-2.113372
10	1	0	-2.437246	-1.031822	-1.127685
11	6	0	-1.468259	-0.433286	1.286304
12	1	0	-1.353518	-1.471955	1.610498
13	1	0	-2.534176	-0.214942	1.180006
14	1	0	-1.059866	0.223411	2.060785
15	6	0	1.347437	-1.109028	1.120201
16	1	0	2.438175	-1.031318	1.126918
17	1	0	1.078924	-2.149771	0.908780
18	1	0	0.980527	-0.844399	2.113773
19	6	0	1.467921	-0.433089	-1.286219
20	1	0	2.533748	-0.214015	-1.180565
21	1	0	1.058705	0.222943	-2.060842
22	1	0	1.353651	-1.471999	-1.609831

Zero-point correction= 0.193626
(Hartree/Particle)
Thermal correction to Energy= 0.202926
Thermal correction to Enthalpy= 0.203871
Thermal correction to Gibbs Free Energy= 0.160815
Sum of electronic and zero-point Energies= -411.489388
Sum of electronic and thermal Energies= -411.480089
Sum of electronic and thermal Enthalpies= -411.479144
Sum of electronic and thermal Free Energies= -411.522200

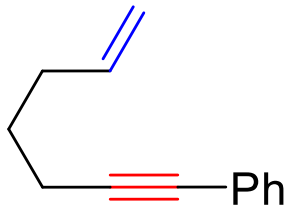
MeBpin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.581059	-0.470592	-0.245033
2	6	0	0.492760	0.497946	0.347612
3	8	0	-0.006477	0.727573	1.679885
4	5	0	-1.360941	0.493649	1.653810
5	8	0	-1.767875	-0.088833	0.478437
6	6	0	-2.324782	0.852775	2.835797
7	6	0	-0.835245	-0.311109	-1.735507
8	1	0	0.077037	-0.517114	-2.305948
9	1	0	-1.181313	0.696371	-1.974698
10	1	0	-1.604754	-1.020552	-2.052569
11	6	0	-0.306862	-1.934781	0.093627

12	1	0	0.549358	-2.323541	-0.465840
13	1	0	-1.190135	-2.526275	-0.161858
14	1	0	-0.110985	-2.056103	1.163676
15	6	0	1.896639	-0.079037	0.435268
16	1	0	2.570843	0.665143	0.868419
17	1	0	2.268760	-0.339849	-0.561540
18	1	0	1.922042	-0.969911	1.065914
19	6	0	0.518482	1.853186	-0.357197
20	1	0	1.129061	2.543703	0.230787
21	1	0	-0.490708	2.269846	-0.435541
22	1	0	0.944971	1.776600	-1.361944
23	1	0	-3.359417	0.582096	2.614822
24	1	0	-2.283518	1.923842	3.058710
25	1	0	-2.018882	0.332968	3.749908

Zero-point correction= 0.221583
(Hartree/Particle)
Thermal correction to Energy= 0.232086
Thermal correction to Enthalpy= 0.233030
Thermal correction to Gibbs Free Energy= 0.187139
Sum of electronic and zero-point Energies= -450.770799
Sum of electronic and thermal Energies= -450.760297
Sum of electronic and thermal Enthalpies= -450.759353
Sum of electronic and thermal Free Energies= -450.805243

Enyne



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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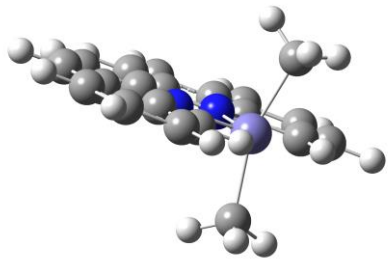
3	6	0	1.725376	-1.149621	0.600930
4	6	0	2.647696	-0.148051	-0.108788
5	6	0	4.125048	-0.520577	0.050551
6	6	0	5.026973	0.430822	-0.681029
7	6	0	5.946001	1.199648	-0.104938
8	6	0	-2.223504	-0.131906	0.110869
9	6	0	-2.650339	1.173251	0.392454
10	6	0	-3.980878	1.530318	0.209412
11	6	0	-4.901189	0.592812	-0.254749
12	6	0	-4.484437	-0.706740	-0.535405
13	6	0	-3.155175	-1.070002	-0.355148
14	1	0	1.979460	-1.187930	1.668019
15	1	0	1.903711	-2.156718	0.203345
16	1	0	2.383616	-0.109961	-1.172121
17	1	0	2.475155	0.855403	0.294938
18	1	0	4.391663	-0.537412	1.114777
19	1	0	4.275613	-1.539978	-0.332514

20	1	0	4.882141	0.489510	-1.760412
21	1	0	6.563555	1.881255	-0.681088
22	1	0	6.115207	1.170407	0.968824
23	1	0	-1.928049	1.897650	0.754351
24	1	0	-4.300538	2.544054	0.430025
25	1	0	-5.939907	0.873796	-0.397730
26	1	0	-5.197725	-1.440265	-0.898234
27	1	0	-2.823392	-2.079908	-0.573092

Zero-point correction= 0.231948
(Hartree/Particle)
Thermal correction to Energy= 0.244739
Thermal correction to Enthalpy= 0.245683
Thermal correction to Gibbs Free Energy= 0.190424
Sum of electronic and zero-point Energies= -503.260591
Sum of electronic and thermal Energies= -503.247800
Sum of electronic and thermal Enthalpies= -503.246855
Sum of electronic and thermal Free Energies= -503.302114

I



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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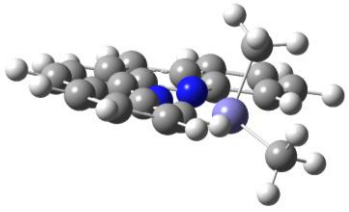
3	6	0	2.880396	-0.000500	2.358537
4	6	0	2.646687	0.000160	-0.061864
5	6	0	1.519962	-0.000296	2.459597
6	6	0	3.491552	-0.000305	1.075879
7	6	0	3.217756	0.000402	-1.355973
8	1	0	1.040384	-0.000429	3.430779
9	1	0	5.535787	-0.000933	1.767935
10	1	0	3.506373	-0.000826	3.246100
11	6	0	4.582640	0.000118	-1.504954
12	1	0	2.561321	0.000882	-2.222001
13	1	0	5.016468	0.000293	-2.499569
14	6	0	5.430164	-0.000378	-0.372894
15	1	0	6.506669	-0.000589	-0.508753
16	6	0	4.894291	-0.000567	0.891167
17	6	0	-0.733057	0.000117	1.276919
18	7	0	-1.284238	0.000523	0.064367
19	6	0	-2.881251	-0.000570	2.358132
20	6	0	-2.647184	0.000421	-0.062224
21	6	0	-1.520835	-0.000405	2.459397

22	6	0	-3.492218	-0.000173	1.075381
23	6	0	-3.218007	0.000895	-1.356428
24	1	0	-1.041422	-0.000721	3.430663
25	1	0	-5.536582	-0.000809	1.767080
26	1	0	-3.507361	-0.001014	3.245602
27	6	0	-4.582863	0.000712	-1.505649
28	1	0	-2.561409	0.001474	-2.222344
29	1	0	-5.016530	0.001081	-2.500334
30	6	0	-5.430576	0.000074	-0.373729
31	1	0	-6.507057	-0.000062	-0.509776
32	6	0	-4.894926	-0.000343	0.890428
33	26	0	-0.000279	0.000485	-1.405697
34	6	0	0.001434	2.009366	-1.776001
35	1	0	0.888615	2.307055	-2.357319
36	1	0	0.000598	2.609198	-0.855899
37	1	0	-0.883185	2.308845	-2.360257
38	6	0	0.000335	-2.009072	-1.771974
39	1	0	0.001261	-2.607174	-0.850730
40	1	0	0.886243	-2.307993	-2.354595
41	1	0	-0.885623	-2.309369	-2.353781

Zero-point correction= (Hartree/Particle)	0.326683
Thermal correction to Energy=	0.347324
Thermal correction to Enthalpy=	0.348268
Thermal correction to Gibbs Free Energy=	0.277538
Sum of electronic and zero-point Energies=	-1005.089516
Sum of electronic and thermal Energies=	-1005.068875
Sum of electronic and thermal Enthalpies=	-1005.067931
Sum of electronic and thermal Free Energies=	-1005.138661

Icis



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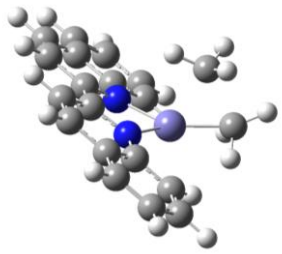
3	6	0	2.851542	-0.113505	2.468884
4	6	0	2.596581	0.037126	0.056145
5	6	0	1.490247	-0.172286	2.576140
6	6	0	3.450384	0.001452	1.192899
7	6	0	3.164996	0.159516	-1.237042
8	1	0	1.019145	-0.242292	3.548285
9	1	0	5.493943	0.056452	1.890650
10	1	0	3.482137	-0.145935	3.353288
11	6	0	4.527356	0.246952	-1.374303
12	1	0	2.491321	0.181695	-2.087096
13	1	0	4.958947	0.344228	-2.365396

14	6	0	5.381303	0.209627	-0.245118
15	1	0	6.455943	0.277666	-0.381148
16	6	0	4.852966	0.087333	1.013932
17	6	0	-0.777626	-0.127472	1.437019
18	7	0	-1.359879	0.020134	0.258211
19	6	0	-2.886630	-0.209035	2.582327
20	6	0	-2.720619	0.092290	0.179818
21	6	0	-1.521431	-0.256739	2.638804
22	6	0	-3.535271	-0.021751	1.337132
23	6	0	-3.329998	0.291981	-1.084991
24	1	0	-1.017641	-0.396272	3.587004
25	1	0	-5.558548	-0.033776	2.095282
26	1	0	-3.484263	-0.308199	3.484199
27	6	0	-4.696368	0.366145	-1.180737
28	1	0	-2.695674	0.400964	-1.959768
29	1	0	-5.159930	0.524956	-2.148955
30	6	0	-5.512046	0.244880	-0.029163
31	1	0	-6.590872	0.306106	-0.128478
32	6	0	-4.943411	0.056148	1.204402
33	26	0	-0.094167	0.033837	-1.376763
34	6	0	-0.174818	1.992195	-1.485905
35	1	0	0.809432	2.372482	-1.790768
36	1	0	-0.464712	2.491299	-0.548926
37	1	0	-0.892293	2.291968	-2.266194
38	6	0	0.539608	-0.369460	-3.264188
39	1	0	1.056386	-1.329514	-3.420608
40	1	0	1.153369	0.420546	-3.720207
41	1	0	-0.376512	-0.416001	-3.882945

Zero-point correction= (Hartree/Particle)	0.327422
Thermal correction to Energy=	0.347862
Thermal correction to Enthalpy=	0.348806
Thermal correction to Gibbs Free Energy=	0.278496
Sum of electronic and zero-point Energies=	-1005.091592
Sum of electronic and thermal Energies=	-1005.071153
Sum of electronic and thermal Enthalpies=	-1005.070209
Sum of electronic and thermal Free Energies=	-1005.140518

TS for C-C reductive elimination from I(Activation G = 32.9 kcal mol^{-1}, 34.1 kcal mol^{-1} from **Icis**)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.712216	1.349378	0.086507

2	7	0	-1.259494	0.127440	-0.169846
3	6	0	-2.876774	2.401937	0.270428
4	6	0	-2.635349	0.030626	-0.282993
5	6	0	-1.524671	2.496597	0.334433
6	6	0	-3.481729	1.146663	-0.066493
7	6	0	-3.221654	-1.201908	-0.633247
8	1	0	-1.051453	3.442484	0.572562
9	1	0	-5.510386	1.856005	-0.015208
10	1	0	-3.512538	3.262056	0.458630
11	6	0	-4.590240	-1.330018	-0.753335
12	1	0	-2.573675	-2.048359	-0.840251
13	1	0	-5.018172	-2.288038	-1.031983
14	6	0	-5.429805	-0.227307	-0.524357
15	1	0	-6.505776	-0.333415	-0.616706
16	6	0	-4.875804	0.990627	-0.189204
17	6	0	0.710964	1.351792	0.083380
18	7	0	1.259442	0.130265	-0.169041
19	6	0	2.875543	2.408222	0.245744
20	6	0	2.634427	0.031692	-0.281619
21	6	0	1.523618	2.501678	0.318831
22	6	0	3.480845	1.150340	-0.081355
23	6	0	3.218581	-1.207459	-0.611128
24	1	0	1.051102	3.449331	0.551239
25	1	0	5.510252	1.859431	-0.046870
26	1	0	3.511110	3.271218	0.421124
27	6	0	4.586662	-1.337655	-0.733702
28	1	0	2.568624	-2.058181	-0.795721
29	1	0	5.014410	-2.300663	-0.994851
30	6	0	5.426635	-0.230765	-0.526441
31	1	0	6.502302	-0.338618	-0.620310
32	6	0	4.874422	0.992259	-0.206871
33	26	0	0.001599	-1.316160	0.044378
34	6	0	0.030061	-1.647244	2.096563
35	1	0	-0.894768	-1.959569	2.582250
36	1	0	0.120254	-0.557727	2.168850
37	1	0	0.887712	-2.097437	2.597145
38	6	0	-0.020965	-3.088222	0.672579
39	1	0	-0.918837	-3.156777	0.014470
40	1	0	-0.073887	-3.847265	1.446489
41	1	0	0.897227	-3.225623	0.061185

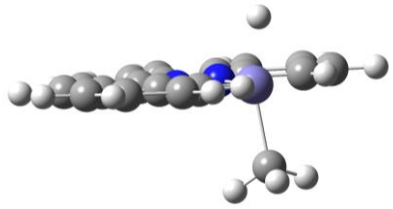
Zero-point correction= 0.327760
(Hartree/Particle)
Thermal correction to Energy= 0.347114
Thermal correction to Enthalpy= 0.348058
Thermal correction to Gibbs Free Energy= 0.279697
Sum of electronic and zero-point Energies= -1005.038139
Sum of electronic and thermal Energies= -1005.018785
Sum of electronic and thermal Enthalpies= -1005.017841
Sum of electronic and thermal Free Energies= -1005.086202

THF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.812350	0.011179	0.048395
2	6	0	0.659064	0.302148	-0.248518
3	6	0	-1.403278	1.421527	0.014323
4	1	0	-0.960363	-0.505420	0.999564
5	1	0	-1.247950	-0.599713	-0.749551
6	1	0	1.170338	-0.525974	-0.749194
7	1	0	1.205067	0.536082	0.676502
8	1	0	-2.482727	1.442692	-0.152584
9	6	0	-0.610668	2.044141	-1.135439
10	1	0	-1.187041	1.944004	0.952351
11	1	0	-0.489579	3.127626	-1.039276
12	1	0	-1.093633	1.835134	-2.100611
13	8	0	0.674119	1.435574	-1.106961

Zero-point correction= 0.118784
(Hartree/Particle)
Thermal correction to Energy= 0.123617
Thermal correction to Enthalpy= 0.124561
Thermal correction to Gibbs Free Energy= 0.090739
Sum of electronic and zero-point Energies= -232.215679
Sum of electronic and thermal Energies= -232.210846
Sum of electronic and thermal Enthalpies= -232.209902
Sum of electronic and thermal Free Energies= -232.243724

II-*trans*

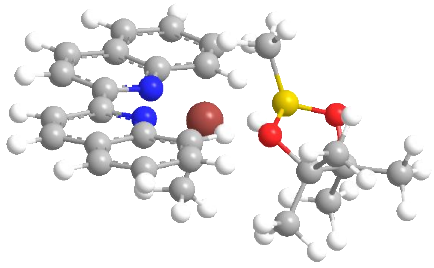


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.737682	-0.005817	1.473259
2	7	0	1.290222	0.015757	0.264011
3	6	0	2.884442	-0.059301	2.555272
4	6	0	2.651556	0.003012	0.137794
5	6	0	1.523188	-0.045966	2.655837
6	6	0	3.496410	-0.034650	1.274284
7	6	0	3.220402	0.021616	-1.157340
8	1	0	1.044037	-0.064912	3.626862
9	1	0	5.542437	-0.078782	1.963863
10	1	0	3.509452	-0.090514	3.443184
11	6	0	4.584219	0.007472	-1.307554
12	1	0	2.560976	0.036826	-2.021310
13	1	0	5.018116	0.018648	-2.301963
14	6	0	5.433106	-0.026494	-0.175788

15	1	0	6.509317	-0.038157	-0.313589
16	6	0	4.899710	-0.048085	1.088436
17	6	0	-0.731041	-0.006244	1.473709
18	7	0	-1.284340	0.015339	0.264813
19	6	0	-2.877094	-0.061561	2.557032
20	6	0	-2.645740	0.001758	0.139433
21	6	0	-1.515790	-0.047324	2.656760
22	6	0	-3.489869	-0.036859	1.276431
23	6	0	-3.215401	0.020465	-1.155339
24	1	0	-1.036019	-0.066363	3.627477
25	1	0	-5.535433	-0.082631	1.967264
26	1	0	-3.501535	-0.093565	3.445315
27	6	0	-4.579300	0.005435	-1.304714
28	1	0	-2.556529	0.036532	-2.019714
29	1	0	-5.013817	0.016681	-2.298852
30	6	0	-5.427466	-0.029532	-0.172436
31	1	0	-6.503754	-0.041893	-0.309579
32	6	0	-4.893273	-0.051190	1.091449
33	26	0	0.002478	0.098823	-1.218432
34	6	0	0.002007	2.109346	-1.492351
35	1	0	0.887026	2.440444	-2.059140
36	1	0	0.002271	2.663672	-0.544134
37	1	0	-0.883414	2.440291	-2.058585
38	1	0	0.002760	-1.541277	-1.462664

Zero-point correction= (Hartree/Particle)	0.297551
Thermal correction to Energy=	0.315854
Thermal correction to Enthalpy=	0.316799
Thermal correction to Gibbs Free Energy=	0.251396
Sum of electronic and zero-point Energies=	-965.818213
Sum of electronic and thermal Energies=	-965.799910
Sum of electronic and thermal Enthalpies=	-965.798965
Sum of electronic and thermal Free Energies=	-965.864368

II

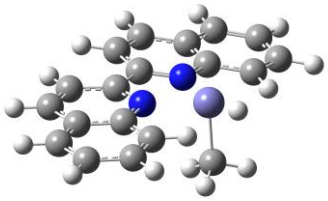


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.083258	-0.247328	-0.019581
2	1	0	0.125356	1.972449	0.135937
3	5	0	-0.798176	2.068481	-0.815266
4	8	0	-1.439214	3.335375	-0.724031
5	6	0	-2.397762	3.232647	0.321203
6	6	0	-2.928914	1.755787	0.184207

7	8	0	-1.818345	1.052665	-0.389390
8	6	0	-0.036605	-0.074394	1.963062
9	1	0	0.811869	-0.672576	2.332474
10	1	0	-0.954779	-0.631281	2.202040
11	1	0	-0.049128	0.859827	2.540102
12	6	0	-0.104386	1.602202	-2.197547
13	1	0	0.354999	0.590250	-2.153066
14	1	0	0.697289	2.276928	-2.515252
15	1	0	-0.856337	1.540401	-2.991834
16	6	0	-1.715263	3.487624	1.670035
17	1	0	-1.215761	4.460070	1.621414
18	1	0	-0.963922	2.726154	1.892206
19	1	0	-2.441757	3.510438	2.488944
20	6	0	-3.468036	4.295129	0.096583
21	1	0	-3.869952	4.240754	-0.917143
22	1	0	-3.025373	5.285993	0.234192
23	1	0	-4.289315	4.183178	0.813670
24	6	0	-3.343110	1.107079	1.496549
25	1	0	-2.510510	1.075396	2.200957
26	1	0	-3.671303	0.077766	1.312538
27	1	0	-4.176006	1.656122	1.951297
28	6	0	-4.059208	1.648703	-0.841455
29	1	0	-3.753147	2.103698	-1.788147
30	1	0	-4.976565	2.132907	-0.491742
31	1	0	-4.278425	0.590972	-1.023831
32	6	0	1.106921	-2.423258	0.085724
33	7	0	-0.045203	-1.821640	-0.166760
34	6	0	0.064163	-4.577213	0.303430
35	6	0	-1.188965	-2.568920	-0.235272
36	6	0	1.198810	-3.816678	0.335325
37	6	0	-1.176101	-3.970453	0.002433
38	6	0	-2.413798	-1.932559	-0.559074
39	1	0	2.150537	-4.272899	0.572548
40	1	0	-2.363822	-5.770738	0.122954
41	1	0	0.102570	-5.644127	0.505743
42	6	0	-3.568890	-2.670495	-0.624278
43	1	0	-2.400502	-0.864657	-0.750662
44	1	0	-4.504164	-2.178293	-0.873814
45	6	0	-3.562507	-4.063895	-0.372107
46	1	0	-4.489867	-4.625147	-0.424780
47	6	0	-2.387913	-4.701341	-0.067211
48	6	0	2.306851	-1.549043	0.093135
49	6	0	4.690029	-1.254850	0.152541
50	6	0	3.149468	0.612734	-0.066123
51	6	0	3.613335	-2.094047	0.182408
52	6	0	4.488026	0.137447	0.022092
53	6	0	2.931616	2.006697	-0.216538
54	1	0	3.760035	-3.163025	0.258151
55	1	0	6.580112	0.669499	0.036634
56	1	0	5.702552	-1.643966	0.216719
57	6	0	3.997371	2.868646	-0.274163
58	1	0	1.913896	2.369092	-0.277614
59	1	0	3.815234	3.932031	-0.391584
60	6	0	5.327793	2.395409	-0.181266
61	1	0	6.154263	3.097106	-0.227103
62	6	0	5.566628	1.054293	-0.034761
63	26	0	0.071907	0.234932	0.009328

Zero-point correction=	0.525611 (Hartree/Particle)
Thermal correction to Energy=	0.555307
Thermal correction to Enthalpy=	0.556251
Thermal correction to Gibbs Free Energy=	0.466803
Sum of electronic and zero-point Energies=	-1416.641043
Sum of electronic and thermal Energies=	-1416.611347
Sum of electronic and thermal Enthalpies=	-1416.610402
Sum of electronic and thermal Free Energies=	-1416.699851

III

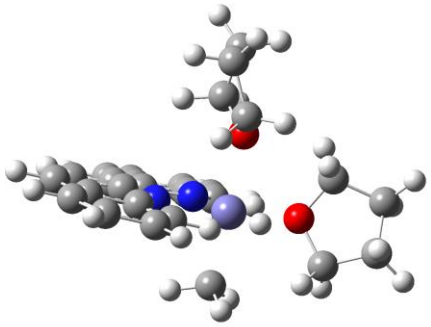


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.743588	1.220160	-0.068393
2	7	0	-1.306830	0.024078	-0.109869
3	6	0	-2.874898	2.327486	-0.010761
4	6	0	-2.665905	-0.088088	-0.074221
5	6	0	-1.510204	2.413977	-0.024457
6	6	0	-3.502335	1.058155	-0.027780
7	6	0	-3.252020	-1.379188	-0.081302
8	1	0	-1.023928	3.381090	-0.013450
9	1	0	-5.540729	1.772858	0.030290
10	1	0	-3.488211	3.223986	0.014117
11	6	0	-4.617102	-1.510024	-0.052825
12	1	0	-2.603963	-2.250929	-0.090563
13	1	0	-5.062802	-2.499434	-0.054078
14	6	0	-5.454437	-0.368013	-0.015873
15	1	0	-6.531838	-0.494955	0.005333
16	6	0	-4.908527	0.889977	-0.001725
17	6	0	0.739565	1.212291	-0.057596
18	7	0	1.304842	0.020244	-0.203205
19	6	0	2.857357	2.313431	0.190565
20	6	0	2.668736	-0.087482	-0.144622
21	6	0	1.493847	2.395841	0.137162
22	6	0	3.490376	1.056763	0.054260
23	6	0	3.272080	-1.365024	-0.272986
24	1	0	0.997742	3.349783	0.262202
25	1	0	5.512903	1.783794	0.272195
26	1	0	3.463091	3.201878	0.348494
27	6	0	4.637321	-1.478841	-0.198732
28	1	0	2.615053	-2.216788	-0.433827
29	1	0	5.096708	-2.457304	-0.296729
30	6	0	5.459248	-0.342389	-0.001666

31	1	0	6.536937	-0.460557	0.050848
32	6	0	4.896951	0.901710	0.119979
33	26	0	-0.000055	-1.558418	-0.347095
34	6	0	-0.070648	-1.986495	1.563994
35	1	0	-0.770790	-2.825378	1.711208
36	1	0	-0.390371	-1.159309	2.215493
37	1	0	0.917314	-2.335442	1.889101
38	1	0	0.793303	-2.910167	-0.892760

Zero-point correction= 0.298541
(Hartree/Particle)
Thermal correction to Energy= 0.316679
Thermal correction to Enthalpy= 0.317624
Thermal correction to Gibbs Free Energy= 0.252303
Sum of electronic and zero-point Energies= -965.818925
Sum of electronic and thermal Energies= -965.800787
Sum of electronic and thermal Enthalpies= -965.799843
Sum of electronic and thermal Free Energies= -965.865163

III·2THF

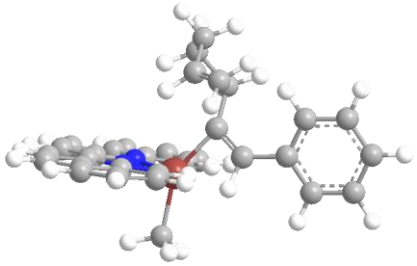


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.441096	-4.081243	0.285059
2	6	0	1.117266	-3.269140	0.049048
3	1	0	2.872653	-4.488587	0.120803
4	6	0	2.460271	-3.495931	-0.040393
5	7	0	1.405874	-0.920333	-0.408879
6	6	0	3.327104	-2.425730	-0.364982
7	6	0	0.616071	-1.954804	-0.155651
8	6	0	2.751409	-1.139247	-0.556285
9	6	0	4.725994	-2.593726	-0.512090
10	1	0	3.093725	0.906237	-1.087938
11	6	0	5.517585	-1.527443	-0.854356
12	1	0	5.152580	-3.581284	-0.357907
13	1	0	6.588832	-1.659987	-0.971317
14	6	0	4.937913	-0.253662	-1.069078
15	1	0	5.572800	0.578112	-1.358657
16	6	0	3.587064	-0.054137	-0.927434
17	7	0	-1.173963	-0.355256	-0.239839
18	1	0	-2.624252	1.062670	-0.387913
19	6	0	-2.436574	-0.002717	-0.259946
20	6	0	-1.804680	-2.652249	-0.001785

21	6	0	-3.504811	-0.927045	-0.141014
22	6	0	-0.841510	-1.677401	-0.115695
23	6	0	-3.175057	-2.299288	-0.005453
24	6	0	-4.863808	-0.527022	-0.156566
25	1	0	-3.970885	-4.302256	0.211486
26	1	0	-1.539495	-3.700982	0.073877
27	6	0	-5.856700	-1.465926	-0.039545
28	1	0	-5.100586	0.527681	-0.266510
29	1	0	-6.898745	-1.163363	-0.052690
30	6	0	-5.530148	-2.838946	0.095399
31	1	0	-6.327977	-3.569449	0.185091
32	6	0	-4.221753	-3.249910	0.111344
33	26	0	0.396992	0.921475	-0.598203
34	1	0	1.635624	2.014307	-0.855636
35	6	0	0.071822	0.504620	-2.587468
36	1	0	0.101164	-0.582785	-2.785698
37	1	0	0.815648	0.964599	-3.253950
38	1	0	-0.924531	0.839083	-2.932037
39	8	0	-0.889362	2.611887	-0.642017
40	6	0	-0.786181	3.497232	0.477021
41	6	0	-1.258505	4.842692	-0.052889
42	6	0	-0.611102	4.832779	-1.439175
43	6	0	-0.759013	3.372357	-1.868556
44	1	0	0.260832	3.542214	0.796903
45	1	0	-1.394207	3.083322	1.287802
46	1	0	-2.351121	4.862439	-0.134279
47	1	0	-0.938717	5.678662	0.574175
48	1	0	0.450157	5.086661	-1.352150
49	1	0	-1.076697	5.523786	-2.145868
50	1	0	0.105337	2.984524	-2.405547
51	1	0	-1.670225	3.199421	-2.450427
52	8	0	0.675194	1.235308	1.515471
53	6	0	-0.042934	0.503331	2.500961
54	6	0	0.547871	0.981571	3.819323
55	6	0	2.033586	1.067201	3.454052
56	6	0	2.001924	1.522353	1.987113
57	1	0	0.115331	-0.577466	2.361327
58	1	0	-1.106070	0.721536	2.369020
59	1	0	0.151801	1.973559	4.062036
60	1	0	0.341439	0.306706	4.653088
61	1	0	2.493709	0.077081	3.535695
62	1	0	2.596462	1.753902	4.090063
63	1	0	2.723427	0.997428	1.356967
64	1	0	2.160413	2.597791	1.866412

Zero-point correction= 0.541111
(Hartree/Particle)
Thermal correction to Energy= 0.570018
Thermal correction to Enthalpy= 0.570962
Thermal correction to Gibbs Free Energy= 0.481290
Sum of electronic and zero-point Energies= -1430.312782
Sum of electronic and thermal Energies= -1430.283875
Sum of electronic and thermal Enthalpies= -1430.282931
Sum of electronic and thermal Free Energies= -1430.372604

IV

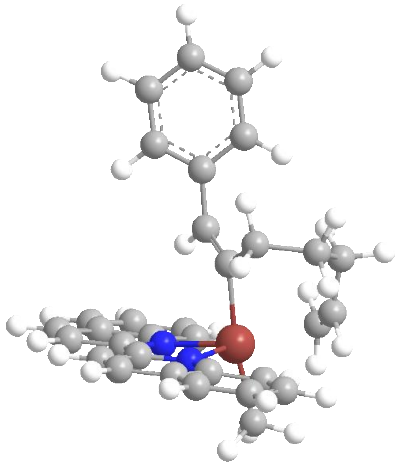


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.492305	0.565450	-1.423652
2	6	0	-0.854868	-0.141506	-2.693367
3	1	0	-0.943155	0.823025	-3.216869
4	1	0	-1.828120	-0.648292	-2.769131
5	1	0	-0.123578	-0.751362	-3.244513
6	6	0	1.764254	1.094626	-0.464719
7	6	0	0.852893	1.069807	0.524919
8	6	0	3.122316	1.668288	-0.578813
9	6	0	5.696973	2.763717	-0.825000
10	6	0	3.584612	2.145613	-1.812314
11	6	0	3.983658	1.725603	0.524637
12	6	0	5.257082	2.273358	0.402233
13	6	0	4.856888	2.692918	-1.934624
14	1	0	2.929512	2.090811	-2.679023
15	1	0	3.655141	1.308415	1.470865
16	1	0	5.912659	2.306816	1.267486
17	1	0	5.195200	3.063518	-2.897668
18	1	0	6.691223	3.189299	-0.919756
19	6	0	0.880079	1.777773	1.843893
20	1	0	0.088993	2.541460	1.792923
21	1	0	1.817166	2.316409	2.046687
22	6	0	0.542212	0.857199	3.023369
23	1	0	0.292255	1.468831	3.898054
24	1	0	-0.356503	0.281508	2.762713
25	6	0	1.667548	-0.107652	3.413907
26	1	0	2.568552	0.459388	3.686012
27	1	0	1.355194	-0.645791	4.320353
28	6	0	2.012435	-1.117965	2.355225
29	1	0	1.166558	-1.614409	1.875799
30	6	0	3.250417	-1.448485	1.996154
31	1	0	3.440330	-2.204967	1.240769
32	1	0	4.119449	-0.972248	2.445330
33	6	0	-2.882807	-0.595894	0.064336
34	7	0	-2.167317	0.495548	-0.195711
35	6	0	-4.884423	0.682501	0.437731
36	6	0	-2.768778	1.726735	-0.154562
37	6	0	-4.263694	-0.531293	0.393761
38	6	0	-4.144813	1.862741	0.158238
39	6	0	-1.999170	2.882615	-0.430765
40	1	0	-4.815729	-1.438850	0.604589
41	1	0	-5.778318	3.248765	0.422201
42	1	0	-5.939828	0.761618	0.682483
43	6	0	-2.589277	4.122641	-0.402568

44	1	0	-0.941093	2.767935	-0.651429
45	1	0	-1.995302	5.005380	-0.615943
46	6	0	-3.962067	4.262580	-0.094974
47	1	0	-4.410620	5.250538	-0.075495
48	6	0	-4.722934	3.153990	0.181843
49	6	0	-2.124106	-1.845726	-0.028472
50	7	0	-0.839135	-1.688776	-0.347229
51	6	0	-1.928689	-4.240427	0.057695
52	6	0	-0.038249	-2.797495	-0.461716
53	6	0	-2.702883	-3.125132	0.185000
54	6	0	-0.554423	-4.105156	-0.272567
55	6	0	1.334288	-2.632558	-0.765751
56	1	0	-3.752203	-3.209593	0.439333
57	1	0	-0.099783	-6.214181	-0.267958
58	1	0	-2.345977	-5.231952	0.208028
59	6	0	2.148668	-3.731918	-0.891483
60	1	0	1.732410	-1.628144	-0.872450
61	1	0	3.200269	-3.595309	-1.123727
62	6	0	1.634335	-5.037271	-0.718519
63	1	0	2.292416	-5.893602	-0.823918
64	6	0	0.308870	-5.217759	-0.411446
65	26	0	-0.324321	0.170513	-0.750354

Zero-point correction= 0.536568 (Hartree/Particle)
Thermal correction to Energy= 0.567944
Thermal correction to Enthalpy= 0.568888
Thermal correction to Gibbs Free Energy= 0.472374
Sum of electronic and zero-point Energies= -1469.149926
Sum of electronic and thermal Energies= -1469.118551
Sum of electronic and thermal Enthalpies= -1469.117607
Sum of electronic and thermal Free Energies= -1469.214121

V



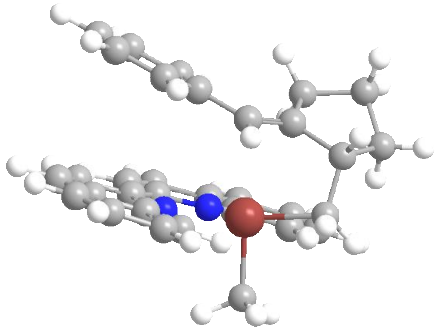
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.098288	0.309447	-0.112566
2	6	0	-1.454594	-2.046812	2.249006

3	1	0	-0.701540	-2.729109	2.676611
4	1	0	-2.041373	-1.665455	3.105319
5	6	0	1.485001	1.216284	-0.156136
6	6	0	0.194113	1.135142	0.226978
7	6	0	2.251644	2.369307	-0.695730
8	6	0	3.801335	4.477928	-1.764651
9	6	0	2.141969	3.677653	-0.201070
10	6	0	3.184150	2.146192	-1.720575
11	6	0	3.944539	3.180602	-2.253249
12	6	0	2.899722	4.718124	-0.731540
13	1	0	1.466455	3.879354	0.625472
14	1	0	3.301027	1.134915	-2.104457
15	1	0	4.653137	2.975788	-3.051048
16	1	0	2.792159	5.720290	-0.326033
17	1	0	4.393893	5.289077	-2.176743
18	6	0	-0.720498	2.339809	0.117837
19	1	0	-1.633696	2.042141	-0.417930
20	1	0	-0.279192	3.147234	-0.478721
21	6	0	-1.148640	2.904442	1.501553
22	1	0	-1.184475	3.998450	1.450729
23	1	0	-2.172840	2.586221	1.742308
24	6	0	-0.239847	2.494289	2.671524
25	1	0	0.816725	2.626681	2.414400
26	1	0	-0.453230	3.148001	3.528980
27	6	0	-0.466661	1.081727	3.127588
28	1	0	-1.510782	0.796271	3.299538
29	6	0	0.480686	0.181239	3.428505
30	1	0	0.219063	-0.787305	3.844200
31	1	0	1.533578	0.422501	3.294902
32	1	0	-2.139550	-2.672960	1.658937
33	6	0	-1.325216	-1.359717	-1.476105
34	7	0	-1.843408	-0.774252	-0.406913
35	6	0	-3.284323	-0.906306	-2.794031
36	6	0	-3.112137	-0.274324	-0.457501
37	6	0	-2.032141	-1.445905	-2.703769
38	6	0	-3.872018	-0.300426	-1.654856
39	6	0	-3.677626	0.281706	0.716027
40	1	0	-1.578807	-1.922591	-3.563583
41	1	0	-5.744653	0.248876	-2.581223
42	1	0	-3.841162	-0.941333	-3.726111
43	6	0	-4.938198	0.821729	0.682451
44	1	0	-3.106135	0.236570	1.638791
45	1	0	-5.369976	1.241912	1.585023
46	6	0	-5.689525	0.822541	-0.517697
47	1	0	-6.684735	1.254938	-0.526986
48	6	0	-5.170181	0.266201	-1.659322
49	6	0	0.023540	-1.914387	-1.271469
50	7	0	0.517004	-1.753685	-0.048605
51	6	0	1.979797	-3.080902	-2.036863
52	6	0	1.739038	-2.290053	0.248055
53	6	0	0.736313	-2.582132	-2.299756
54	6	0	2.520835	-2.953930	-0.734345
55	6	0	2.238392	-2.183850	1.569266
56	1	0	0.302309	-2.684179	-3.286307
57	1	0	4.384484	-3.965119	-1.142386
58	1	0	2.556337	-3.582168	-2.809201
59	6	0	3.471277	-2.694837	1.885485

60	1	0	1.608840	-1.715371	2.315188
61	1	0	3.844119	-2.613331	2.901432
62	6	0	4.262573	-3.334829	0.901990
63	1	0	5.237784	-3.728288	1.169759
64	6	0	3.793606	-3.465231	-0.379943
65	26	0	-0.599338	-0.540136	1.128246

Zero-point correction= 0.537055 (Hartree/Particle)
Thermal correction to Energy= 0.568202
Thermal correction to Enthalpy= 0.569146
Thermal correction to Gibbs Free Energy= 0.474174
Sum of electronic and zero-point Energies= -1469.151000
Sum of electronic and thermal Energies= -1469.119852
Sum of electronic and thermal Enthalpies= -1469.118908
Sum of electronic and thermal Free Energies= -1469.213880

VI

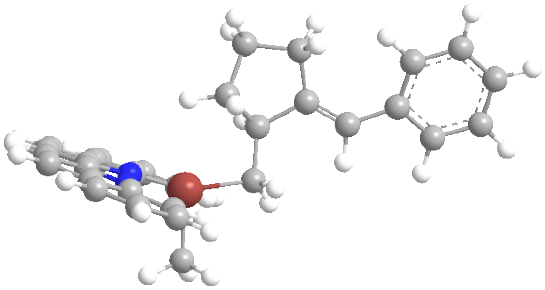


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.401672	-1.644979	-2.737136
2	1	0	-0.029643	-0.855086	-3.372280
3	1	0	-0.115947	-2.586979	-2.979930
4	1	0	1.451342	-1.780754	-3.035752
5	6	0	1.147598	-3.014625	-0.245651
6	1	0	1.997154	-3.423587	-0.807178
7	1	0	0.320426	-3.731577	-0.393068
8	6	0	1.462870	-2.856816	1.248008
9	6	0	2.964589	-2.814601	1.589672
10	6	0	3.086417	-1.812729	2.740420
11	6	0	2.093456	-0.710098	2.342140
12	6	0	0.953538	-1.482561	1.714495
13	1	0	0.987746	-3.621262	1.884979
14	1	0	3.519553	-2.436420	0.721886
15	1	0	3.362533	-3.804864	1.828064
16	1	0	2.761916	-2.274918	3.680643
17	1	0	4.101375	-1.432031	2.886099
18	1	0	2.563125	-0.048501	1.599230
19	1	0	1.767316	-0.086829	3.180543
20	6	0	-0.345028	-1.112907	1.621388
21	1	0	-1.055713	-1.881935	1.305217
22	6	0	-0.967114	0.161804	2.019593

23	6	0	-2.293406	2.551809	2.723578
24	6	0	-2.355191	0.190898	2.229470
25	6	0	-0.263314	1.370809	2.146378
26	6	0	-0.919305	2.547626	2.498118
27	6	0	-3.010130	1.365017	2.581279
28	1	0	-2.923797	-0.728694	2.106092
29	1	0	0.800302	1.402960	1.935833
30	1	0	-0.349557	3.468560	2.586993
31	1	0	-4.084987	1.353537	2.738092
32	1	0	-2.802188	3.470452	2.999329
33	6	0	-1.138665	1.294042	-0.958103
34	7	0	-1.382777	-0.002278	-1.037604
35	6	0	-3.472301	1.837011	-0.846895
36	6	0	-2.671302	-0.444687	-1.051569
37	6	0	-2.173004	2.260360	-0.866805
38	6	0	-3.764726	0.453988	-0.941037
39	6	0	-2.917320	-1.838052	-1.153614
40	1	0	-1.938035	3.313515	-0.776312
41	1	0	-5.914845	0.630296	-0.818024
42	1	0	-4.287441	2.548850	-0.748547
43	6	0	-4.206267	-2.307485	-1.119215
44	1	0	-2.068513	-2.505269	-1.278600
45	1	0	-4.394022	-3.373346	-1.199944
46	6	0	-5.298959	-1.415536	-0.989193
47	1	0	-6.310306	-1.808125	-0.961441
48	6	0	-5.083123	-0.063099	-0.908493
49	6	0	0.300202	1.642671	-0.949777
50	7	0	1.121240	0.603092	-0.948043
51	6	0	2.116258	3.214968	-0.932214
52	6	0	2.470559	0.813796	-0.997148
53	6	0	0.769071	2.981649	-0.942062
54	6	0	3.018853	2.123648	-0.966714
55	6	0	3.335345	-0.306970	-1.082567
56	1	0	0.067907	3.806855	-0.937958
57	1	0	4.838541	3.289629	-0.953244
58	1	0	2.506502	4.228996	-0.911878
59	6	0	4.694087	-0.115939	-1.101271
60	1	0	2.878826	-1.291581	-1.138164
61	1	0	5.355484	-0.974343	-1.166471
62	6	0	5.247205	1.187159	-1.043624
63	1	0	6.324965	1.314032	-1.057202
64	6	0	4.426786	2.284614	-0.983355
65	26	0	0.263255	-1.247384	-0.801771

Zero-point correction= 0.537437 (Hartree/Particle)
Thermal correction to Energy= 0.567701
Thermal correction to Enthalpy= 0.568645
Thermal correction to Gibbs Free Energy= 0.475991
Sum of electronic and zero-point Energies= -1469.195999
Sum of electronic and thermal Energies= -1469.165735
Sum of electronic and thermal Enthalpies= -1469.164791
Sum of electronic and thermal Free Energies= -1469.257445

VII

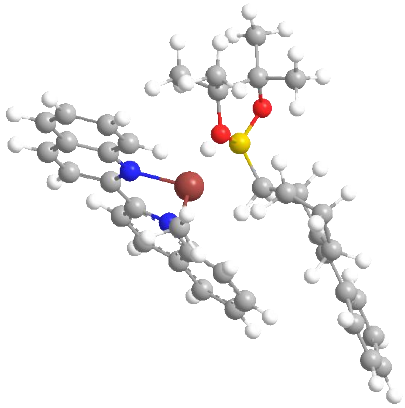


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.460618	-0.073580	-2.673849
2	1	0	-2.548911	-0.147873	-2.821885
3	1	0	-0.985255	-0.882945	-3.250764
4	1	0	-1.117288	0.872489	-3.114847
5	6	0	1.099733	-0.047663	-1.064382
6	1	0	1.546284	0.592906	-1.837390
7	1	0	1.383098	-1.083502	-1.342511
8	6	0	1.664005	0.238989	0.324163
9	6	0	0.858863	-0.438817	1.453176
10	6	0	1.749471	-0.278013	2.687666
11	6	0	3.162952	-0.548214	2.136854
12	6	0	3.097113	-0.169303	0.667217
13	1	0	1.592517	1.326483	0.513523
14	1	0	0.733547	-1.506905	1.215627
15	1	0	-0.143126	0.000578	1.590785
16	1	0	1.679732	0.753743	3.051559
17	1	0	1.484957	-0.941563	3.515436
18	1	0	3.400843	-1.616185	2.234901
19	1	0	3.939555	0.000693	2.681436
20	6	0	4.075023	-0.193800	-0.248109
21	1	0	3.779783	0.091845	-1.258086
22	6	0	5.499912	-0.530461	-0.114911
23	6	0	8.265383	-1.109641	-0.038526
24	6	0	6.330905	-0.295796	-1.223295
25	6	0	6.096744	-1.075666	1.033834
26	6	0	7.458530	-1.359473	1.068005
27	6	0	7.690804	-0.575433	-1.189557
28	1	0	5.889417	0.118383	-2.126211
29	1	0	5.499037	-1.294872	1.908851
30	1	0	7.891098	-1.782872	1.969954
31	1	0	8.303171	-0.376647	-2.064287
32	1	0	9.327499	-1.331763	-0.005860
33	6	0	-3.498353	-0.154969	0.509308
34	7	0	-2.700458	-0.980690	-0.147208
35	6	0	-5.015919	-1.924066	1.087257
36	6	0	-3.026095	-2.301287	-0.247530
37	6	0	-4.681406	-0.599314	1.154557
38	6	0	-4.192158	-2.825728	0.369937
39	6	0	-2.179754	-3.163489	-0.989968
40	1	0	-5.308846	0.095665	1.698339
41	1	0	-5.372406	-4.602168	0.722753

42	1	0	-5.912610	-2.296047	1.575509
43	6	0	-2.486105	-4.496479	-1.093182
44	1	0	-1.310468	-2.739698	-1.484784
45	1	0	-1.840604	-5.154033	-1.666249
46	6	0	-3.641650	-5.025771	-0.467653
47	1	0	-3.863702	-6.083781	-0.561559
48	6	0	-4.479557	-4.207482	0.245911
49	6	0	-3.062878	1.262370	0.494407
50	7	0	-1.908294	1.489621	-0.119261
51	6	0	-3.391317	3.590205	0.979135
52	6	0	-1.457346	2.775057	-0.245533
53	6	0	-3.838481	2.301004	1.066780
54	6	0	-2.179039	3.869171	0.306123
55	6	0	-0.252819	3.020770	-0.952616
56	1	0	-4.775229	2.078633	1.561769
57	1	0	-2.227743	6.010855	0.589002
58	1	0	-3.961479	4.408053	1.411607
59	6	0	0.206983	4.306779	-1.084364
60	1	0	0.264008	2.167540	-1.380104
61	1	0	1.127577	4.492544	-1.628233
62	6	0	-0.500075	5.397681	-0.522330
63	1	0	-0.111761	6.404638	-0.636060
64	6	0	-1.670912	5.183537	0.157812
65	26	0	-0.905887	-0.170901	-0.796729

Zero-point correction= 0.538072 (Hartree/Particle)
Thermal correction to Energy= 0.568572
Thermal correction to Enthalpy= 0.569517
Thermal correction to Gibbs Free Energy= 0.473008
Sum of electronic and zero-point Energies= -1469.173787
Sum of electronic and thermal Energies= -1469.143286
Sum of electronic and thermal Enthalpies= -1469.142342
Sum of electronic and thermal Free Energies= -1469.238850

VIII



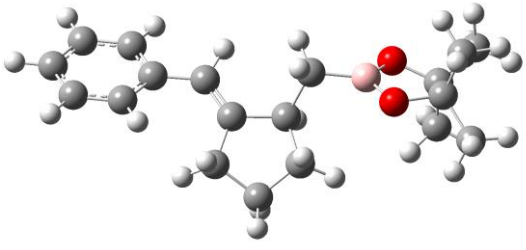
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.299742	2.954851	-0.516947
2	7	0	0.283055	2.207758	-0.107222
3	6	0	-0.148809	4.547258	-1.573802

4	6	0	-0.995027	2.657047	-0.301213
5	6	0	1.121059	4.141386	-1.269427
6	6	0	-1.255735	3.825582	-1.070807
7	6	0	-2.086734	1.977973	0.299753
8	1	0	1.979197	4.694926	-1.629521
9	1	0	-2.777170	5.118115	-1.896247
10	1	0	-0.321367	5.431941	-2.180860
11	6	0	-3.371558	2.408891	0.085528
12	1	0	-1.890222	1.141041	0.956886
13	1	0	-4.197277	1.881784	0.553675
14	6	0	-3.633012	3.532988	-0.734892
15	1	0	-4.658806	3.845392	-0.902268
16	6	0	-2.595031	4.234542	-1.290723
17	6	0	2.641998	2.490297	-0.085176
18	7	0	2.686468	1.269985	0.425777
19	6	0	4.949281	2.900403	0.433371
20	6	0	3.830105	0.828265	1.026766
21	6	0	3.774706	3.342212	-0.109676
22	6	0	5.007282	1.623201	1.038666
23	6	0	3.838457	-0.444365	1.654179
24	1	0	3.702027	4.337867	-0.528554
25	1	0	7.073670	1.735737	1.662287
26	1	0	5.835478	3.528915	0.430057
27	6	0	4.984358	-0.893543	2.259845
28	1	0	2.930151	-1.037808	1.625465
29	1	0	4.988445	-1.865654	2.743370
30	6	0	6.165492	-0.109885	2.262465
31	1	0	7.060558	-0.490547	2.743693
32	6	0	6.177103	1.122420	1.663539
33	26	0	0.948107	0.271406	0.258505
34	6	0	0.683281	0.317376	2.241754
35	1	0	1.236330	1.138384	2.721475
36	1	0	1.014170	-0.620165	2.714541
37	1	0	-0.375073	0.448146	2.520145
38	6	0	-0.906615	-1.032197	-0.579382
39	1	0	-1.513085	-0.524007	-1.339066
40	1	0	-0.888377	-0.312646	0.269569
41	6	0	-1.644393	-2.239569	-0.003822
42	6	0	-0.987858	-2.857578	1.242258
43	6	0	-2.120327	-3.662774	1.880324
44	6	0	-3.324991	-2.716813	1.759835
45	6	0	-3.065401	-1.933990	0.485813
46	1	0	-1.704911	-3.013361	-0.786766
47	1	0	-0.675843	-2.047028	1.915108
48	1	0	-0.094375	-3.441315	1.014225
49	1	0	-2.301740	-4.575348	1.299139
50	1	0	-1.918512	-3.959102	2.913186
51	1	0	-3.333984	-2.032503	2.620056
52	1	0	-4.292478	-3.230736	1.747101
53	6	0	-3.892153	-1.086368	-0.144219
54	1	0	-3.522534	-0.635352	-1.064695
55	6	0	-5.255698	-0.652829	0.198336
56	6	0	-7.856162	0.328167	0.701501
57	6	0	-5.982844	0.038313	-0.786805
58	6	0	-5.865460	-0.825904	1.451579
59	6	0	-7.147907	-0.342188	1.695041
60	6	0	-7.263317	0.518418	-0.545428

61	1	0	-5.521959	0.195994	-1.759055
62	1	0	-5.332443	-1.323292	2.251925
63	1	0	-7.593970	-0.486351	2.674692
64	1	0	-7.799524	1.042630	-1.331037
65	1	0	-8.855835	0.703120	0.897471
66	1	0	0.973326	-0.043160	-1.547790
67	5	0	0.547634	-1.271468	-1.256606
68	8	0	1.523615	-1.796591	-0.251926
69	6	0	2.513641	-2.480308	-1.040467
70	6	0	1.633830	-3.097315	-2.182039
71	8	0	0.649681	-2.102061	-2.416704
72	6	0	3.536279	-1.493910	-1.609748
73	1	0	4.038643	-0.971627	-0.793370
74	1	0	3.055980	-0.754876	-2.257510
75	1	0	4.299937	-2.022700	-2.188689
76	6	0	3.211336	-3.514655	-0.168263
77	1	0	2.483206	-4.109509	0.388546
78	1	0	3.876050	-3.020711	0.547779
79	1	0	3.820488	-4.186974	-0.783258
80	6	0	2.390869	-3.356779	-3.480851
81	1	0	2.769590	-2.425759	-3.907150
82	1	0	1.710426	-3.808924	-4.208541
83	1	0	3.229174	-4.045429	-3.322544
84	6	0	0.926843	-4.383877	-1.746444
85	1	0	0.414090	-4.241585	-0.791416
86	1	0	1.621398	-5.225816	-1.652398
87	1	0	0.175406	-4.634373	-2.501121

Zero-point correction=	0.736744 (Hartree/Particle)
Thermal correction to Energy=	0.776469
Thermal correction to Enthalpy=	0.777413
Thermal correction to Gibbs Free Energy=	0.664814
Sum of electronic and zero-point Energies=	-1880.714658
Sum of electronic and thermal Energies=	-1880.674933
Sum of electronic and thermal Enthalpies=	-1880.673989
Sum of electronic and thermal Free Energies=	-1880.786587

Borylation product (2ea)



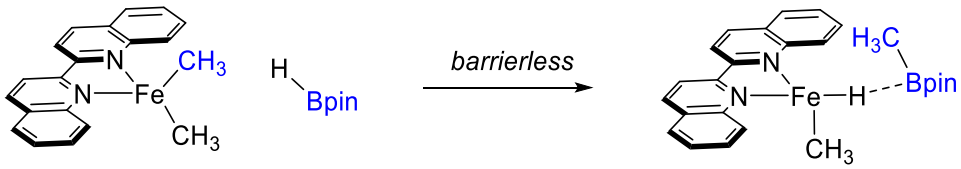
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.470340	-0.430757	-0.742703
2	1	0	0.079391	-1.452254	-0.683066

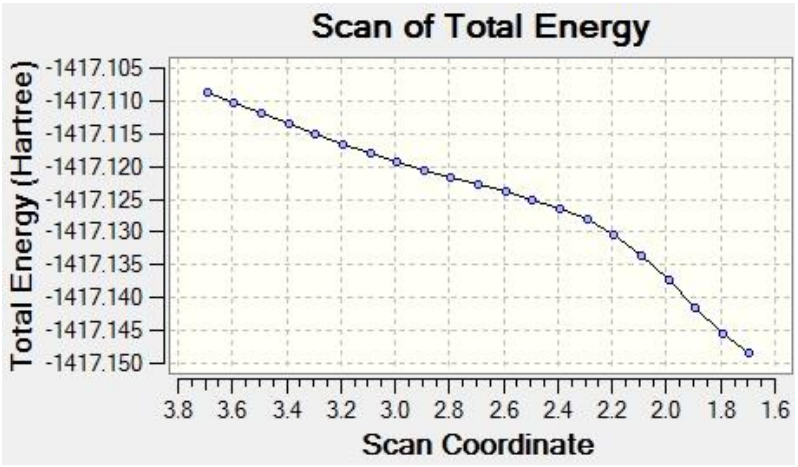
3	1	0	0.233123	-0.040232	-1.739251
4	6	0	-0.224661	0.454793	0.308629
5	6	0	0.247013	1.920727	0.294376
6	6	0	-0.925413	2.690214	0.906133
7	6	0	-2.148444	2.013997	0.269365
8	6	0	-1.743090	0.557634	0.157601
9	1	0	-0.014682	0.036428	1.305687
10	1	0	0.404803	2.239344	-0.744801
11	1	0	1.194265	2.069318	0.821590
12	1	0	-0.942924	2.540820	1.992393
13	1	0	-0.885736	3.766083	0.716418
14	1	0	-2.310998	2.438352	-0.731816
15	1	0	-3.077275	2.150091	0.832523
16	6	0	-2.537513	-0.512000	0.028268
17	1	0	-2.059729	-1.492669	0.038699
18	6	0	-4.006105	-0.551314	-0.067272
19	6	0	-6.814067	-0.735059	-0.183505
20	6	0	-4.677545	-1.698890	0.380179
21	6	0	-4.774937	0.492360	-0.601270
22	6	0	-6.162485	0.401287	-0.655093
23	6	0	-6.063029	-1.789714	0.330962
24	1	0	-4.095489	-2.525412	0.780391
25	1	0	-4.283372	1.369768	-1.006381
26	1	0	-6.736422	1.220483	-1.078181
27	1	0	-6.557892	-2.686398	0.691961
28	1	0	-7.896585	-0.803334	-0.226764
29	5	0	2.018835	-0.435482	-0.488817
30	8	0	2.873044	0.538071	-0.945704
31	6	0	4.214112	0.122577	-0.616826
32	6	0	3.974910	-0.860670	0.574922
33	8	0	2.655790	-1.369475	0.292380
34	6	0	4.779246	-0.572842	-1.853896
35	1	0	4.723021	0.115998	-2.700950
36	1	0	4.196452	-1.465881	-2.100506
37	1	0	5.823774	-0.864902	-1.708585
38	6	0	5.042292	1.351188	-0.275742
39	1	0	4.562937	1.949525	0.501737
40	1	0	5.153446	1.975390	-1.166775
41	1	0	6.041192	1.059808	0.066730
42	6	0	4.952506	-2.022145	0.652115
43	1	0	4.913102	-2.637243	-0.248817
44	1	0	4.701497	-2.653779	1.508718
45	1	0	5.975862	-1.654354	0.784831
46	6	0	3.889651	-0.147183	1.922976
47	1	0	3.188810	0.693001	1.873576
48	1	0	4.865625	0.229106	2.243963
49	1	0	3.522259	-0.853641	2.672053

Zero-point correction= 0.432789
(Hartree/Particle)
Thermal correction to Energy= 0.454012
Thermal correction to Enthalpy= 0.454956
Thermal correction to Gibbs Free Energy= 0.381138
Sum of electronic and zero-point Energies= -914.848180
Sum of electronic and thermal Energies= -914.826957
Sum of electronic and thermal Enthalpies= -914.826013
Sum of electronic and thermal Free Energies= -914.899831

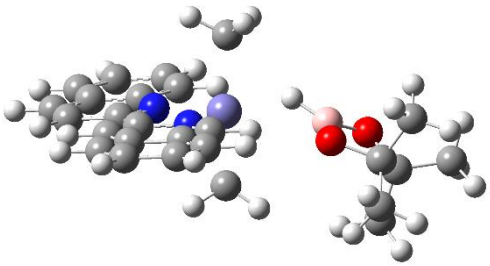
- **Scans of total energy**

Scanning of the potential energy surface through CH_3-B distance for generation of active species

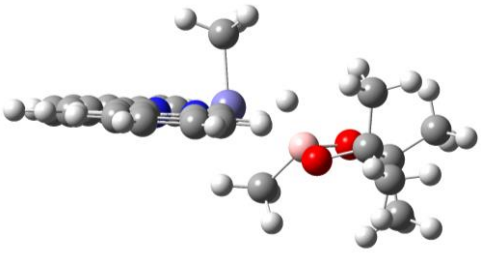




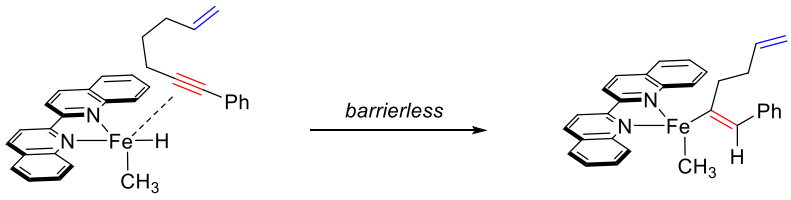
Initial point

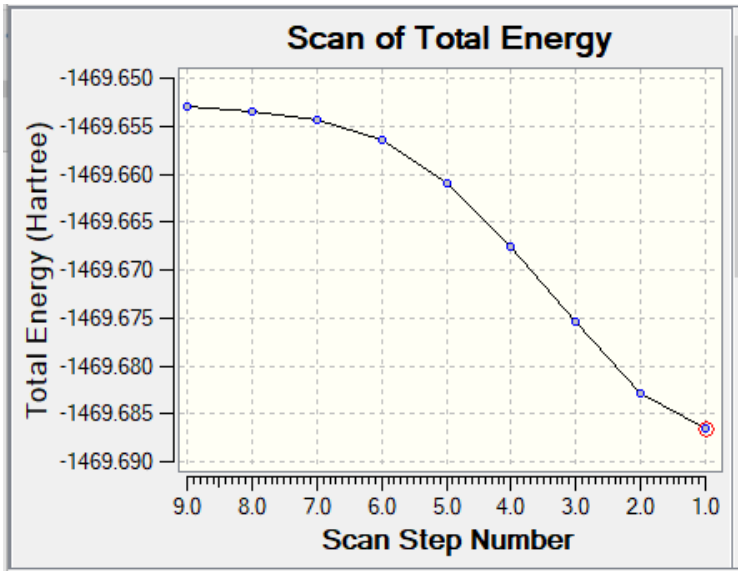


Final point



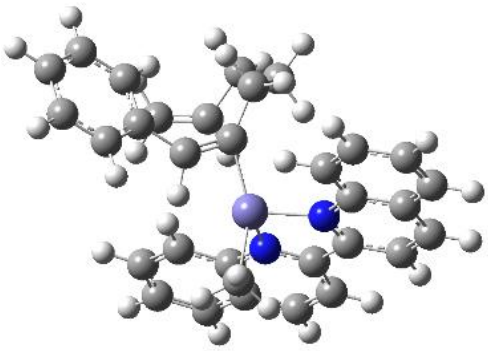
Scanning of the potential energy surface for the hydrometalation of the alkyne



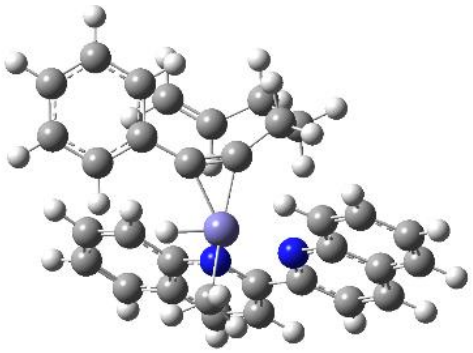


Barrierless

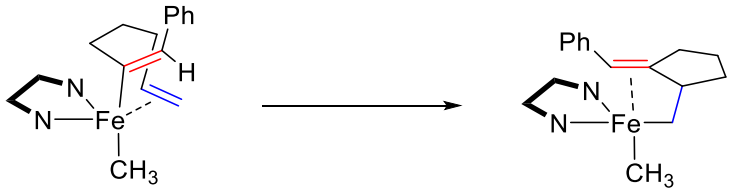
Point 1

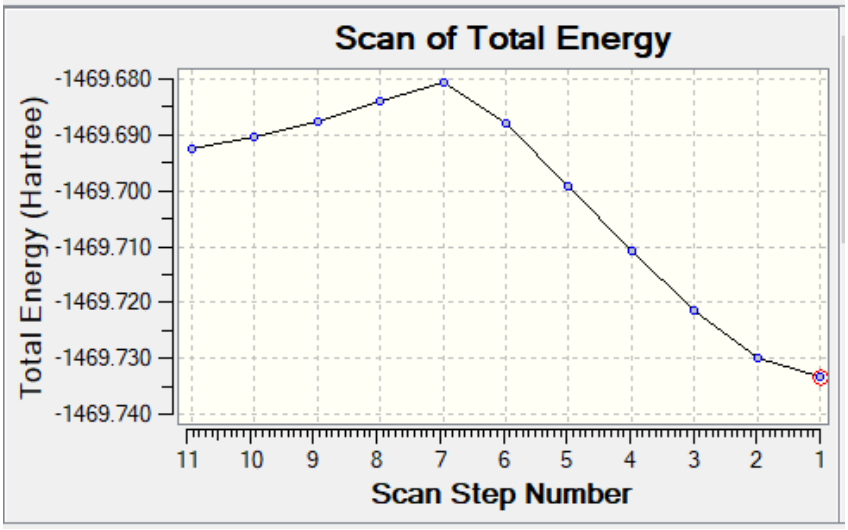


Point 9

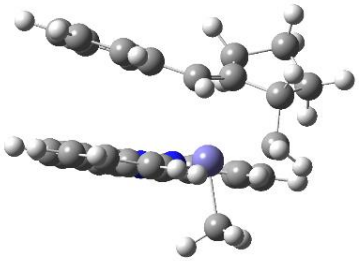


Scanning of the potential energy surface for alkene carbometalation from alkenyl-Fe complex

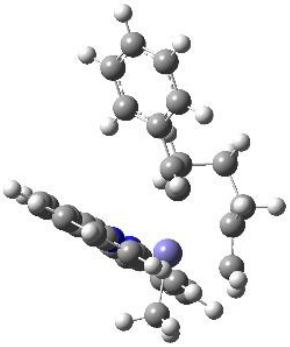




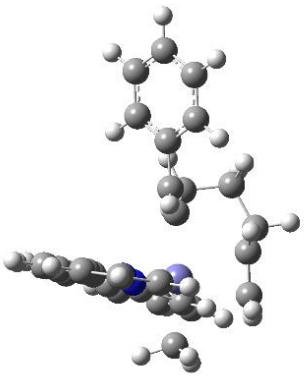
Point 1



Point 7



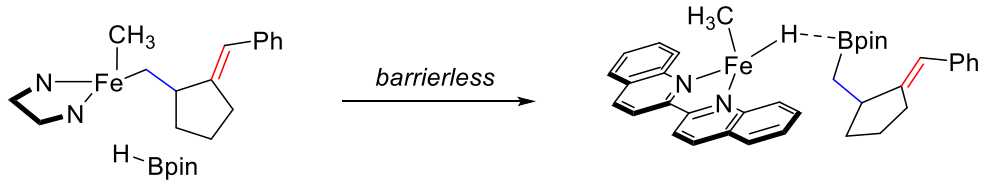
Point 11

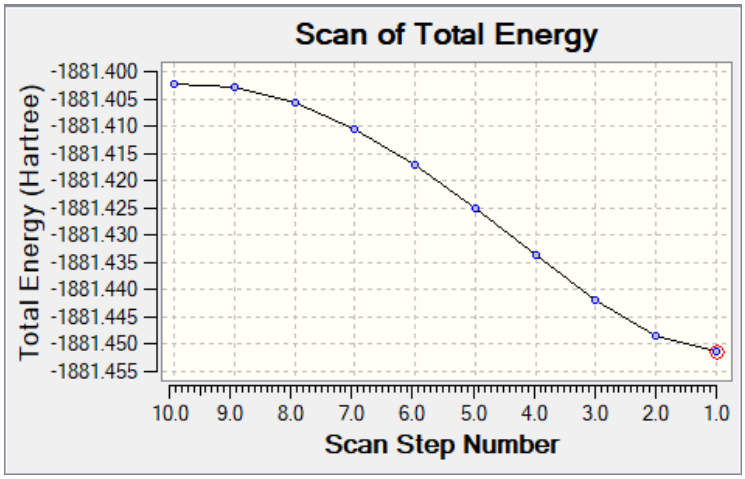


Compound **V** (alkenyl-Fe complex with coordinated alkene) Electronic E = -1469.688055

Point 7, Electronic E = -1469.680566 => **Activation energy around 4.7 kcal mol^{-1}**

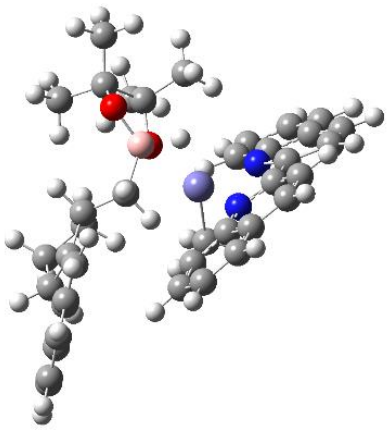
Scanning of the potential energy surface for cleavage of the final alkyl-Fe complex with H-Bpin



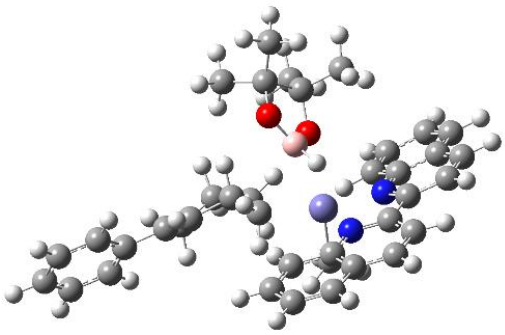


Barrierless

Point 1



Point 10



Alkyl-Fe bond cleavage by HBpin takes place exothermically with no barrier through σ–bond metathesis to re-generate active LFe(H)Me species.

Computational results: Chapter 3

- ***Computational methods***

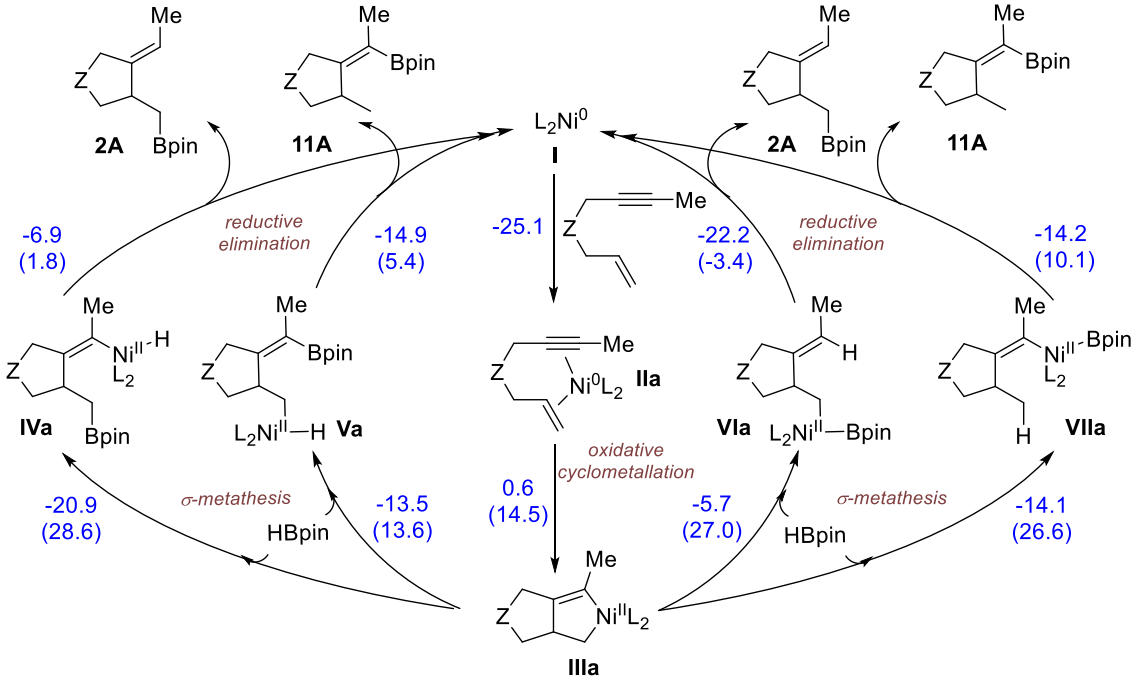
Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the M06-2X hybrid functional[2] that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, N, O, B and P. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set, was used for Ni.[3] Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Gibbs free energy has been used throughout the schemes. The starting approximate geometries for the transition states (TS) were graphically located. Intrinsic reaction coordinate (IRC) studies were performed to confirm the relation of the transition states with the corresponding minima. Solvent effects were considered by performing optimizations in Toluene using the polarized continuum model (PCM).

[1] Gaussian 09, Revision E.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**.

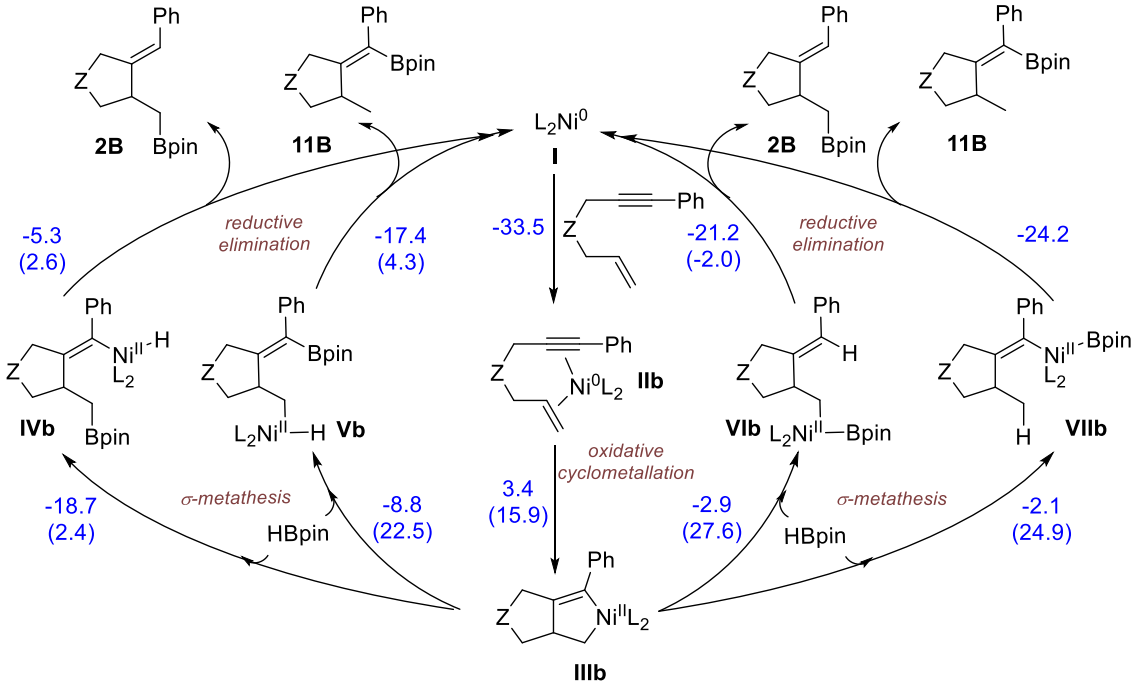
[2] Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, *120*: 215–241.

[3] (a) A. D, Becke, *J. Chem. Phys*. **1993**, *98*, 5648–5653. (b) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098–3100. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785–789.

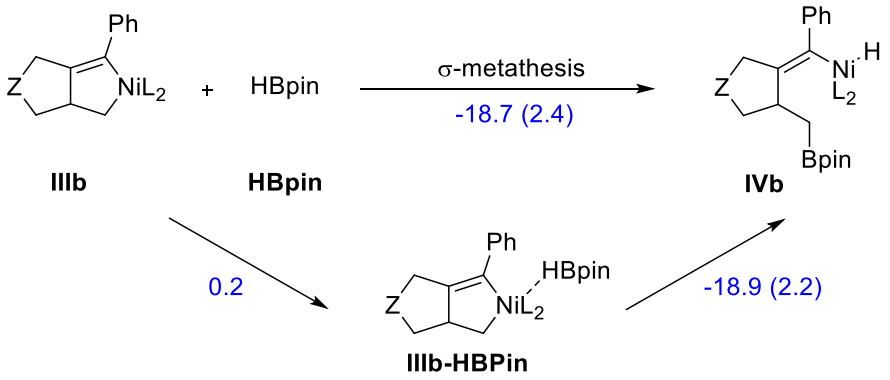
- ***Computed feasible reaction pathways***



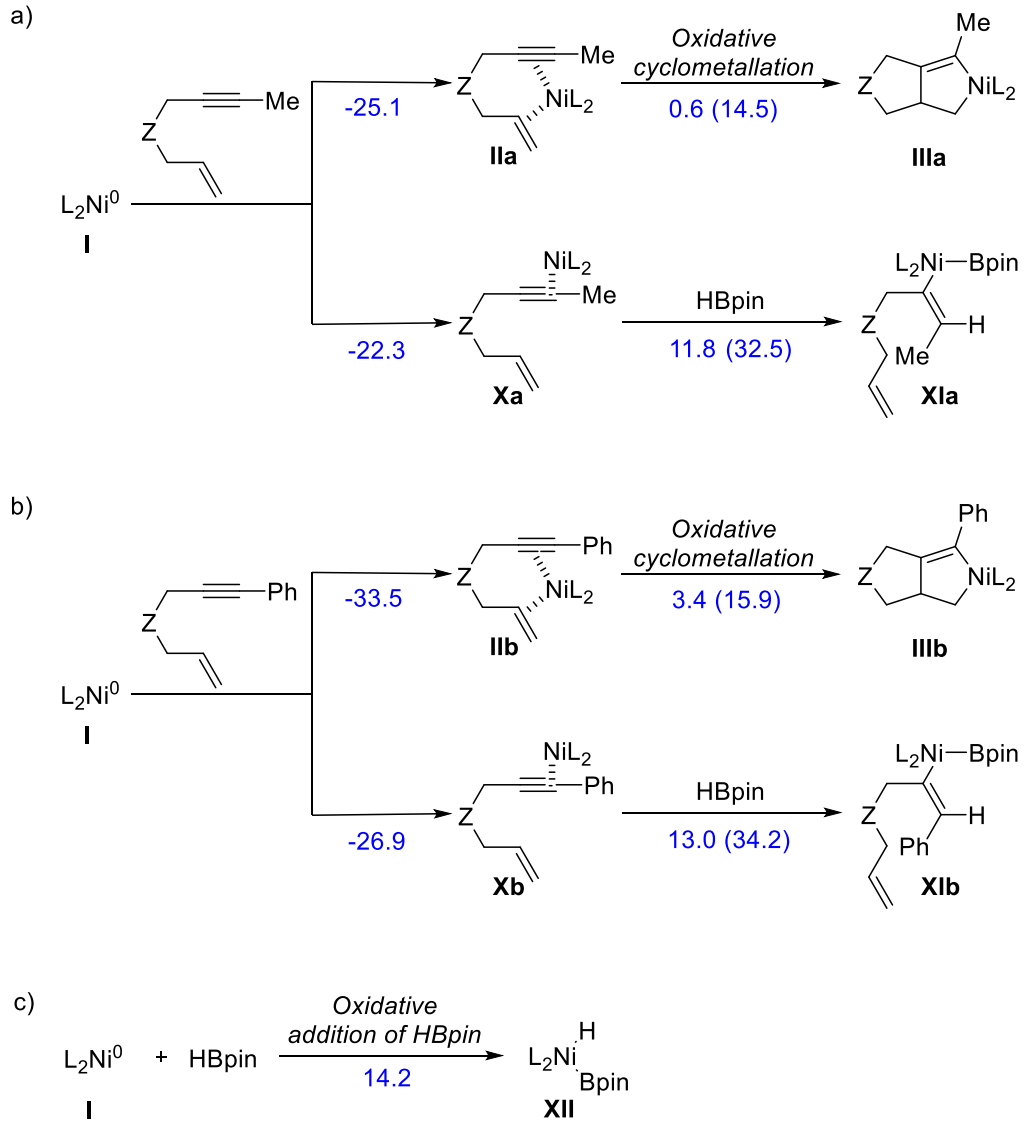
Supplementary Scheme 1. Computed feasible reaction pathways for enyne **I**. ΔG (kcal mol^{-1}) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L_2=Xantphos.



Supplementary Scheme 2. Computed feasible reaction pathways for enyne **I'**. ΔG (kcal mol^{-1}) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L_2=Xantphos.

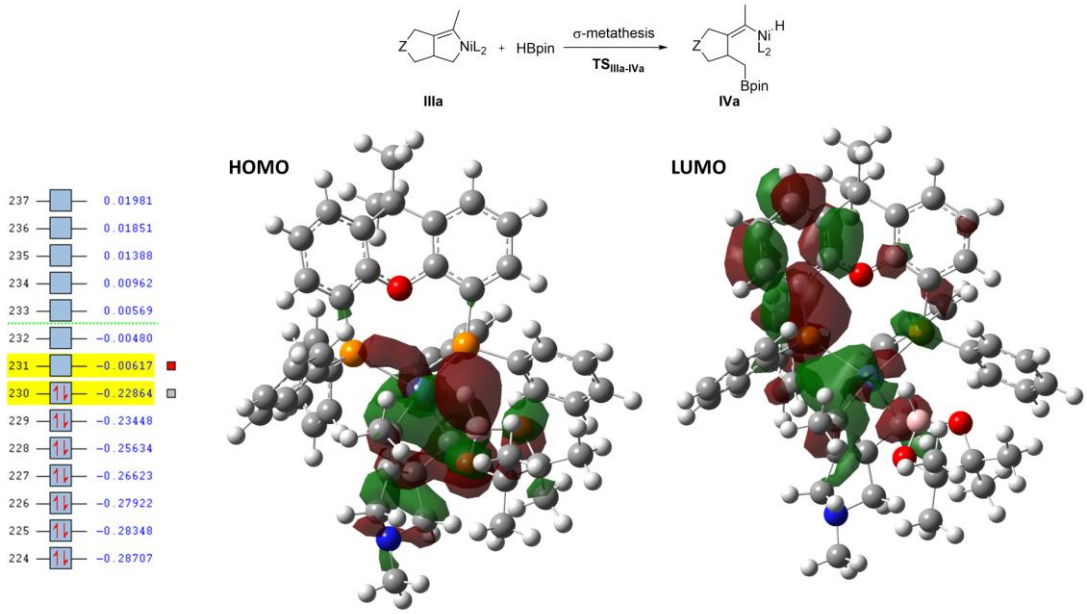


Supplementary Scheme 3. Computed assotiation complex between **IIIb** and HBpin. ΔG (kcal mol^{-1}) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L_2=Xantphos.

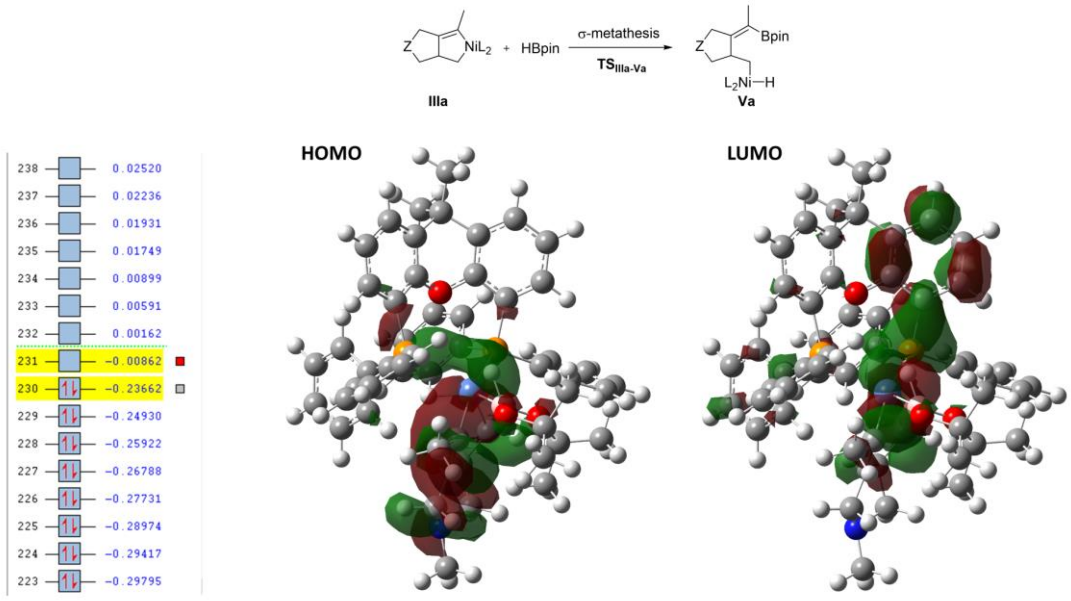


Supplementary Scheme 4. Computed alternative disregarded reaction pathways. ΔG (kcal mol^{-1}) are calculated in toluene (PCM) at 6-31G(d) (C,H,N,P,O,B), LANL2DZ (Ni) level. Calculated activation energies in toluene are shown in brackets. Z= NMe, L_2=Xantphos.

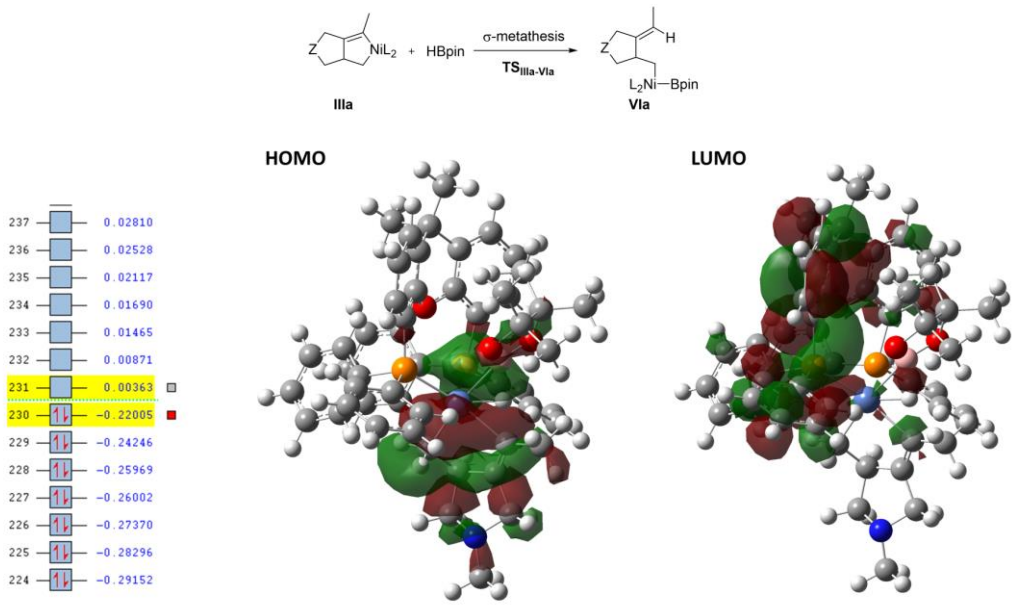
- ***Frontier Orbitals for the σ-metathesis step transition states***



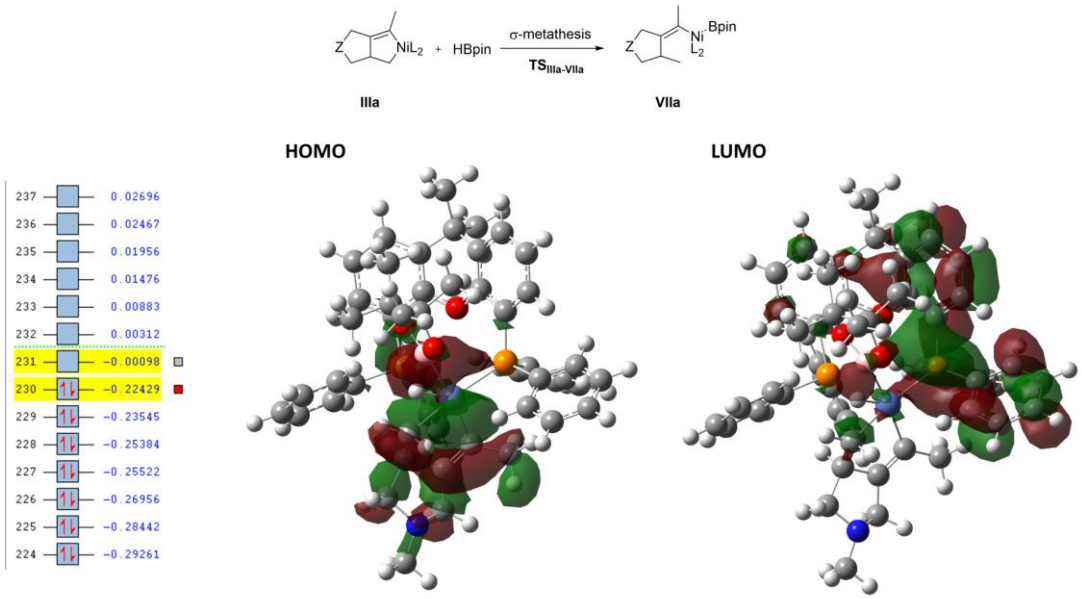
Supplementary Scheme 5. Frontier orbitals for **$TS_{IIIa-IVa}$**



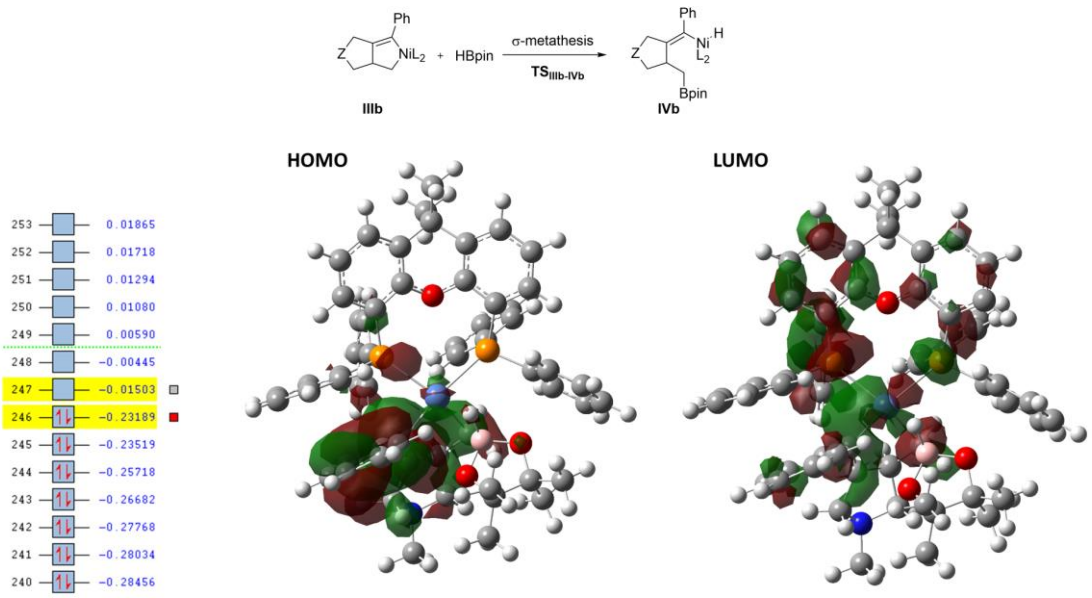
Supplementary Scheme 6. Frontier orbitals for **$TS_{IIIa-Va}$**



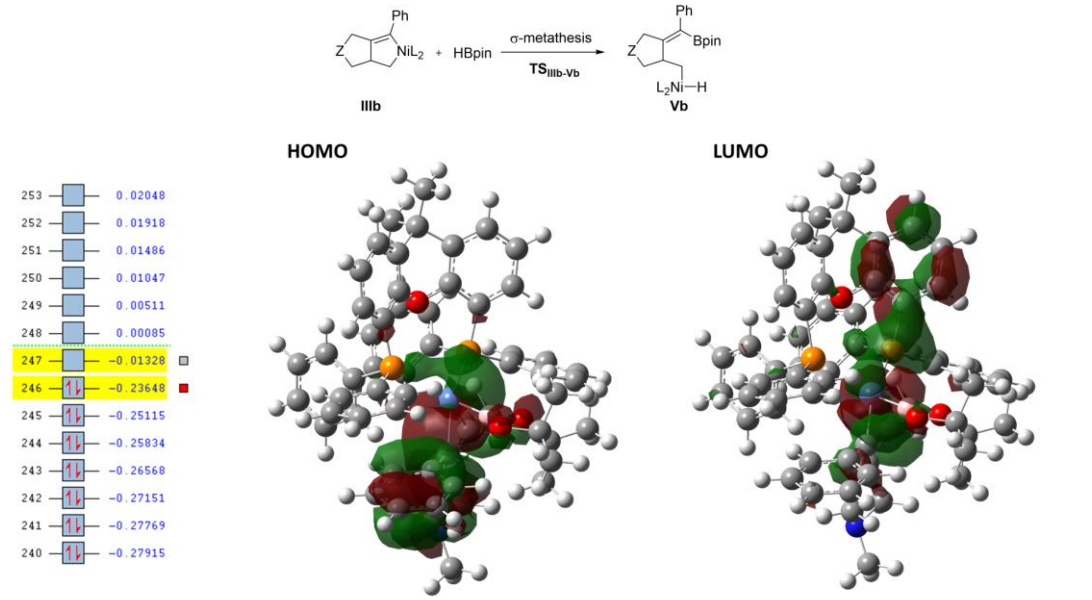
Supplementary Scheme 7. Frontier orbitals for **$TS_{IIIa-VIa}$**



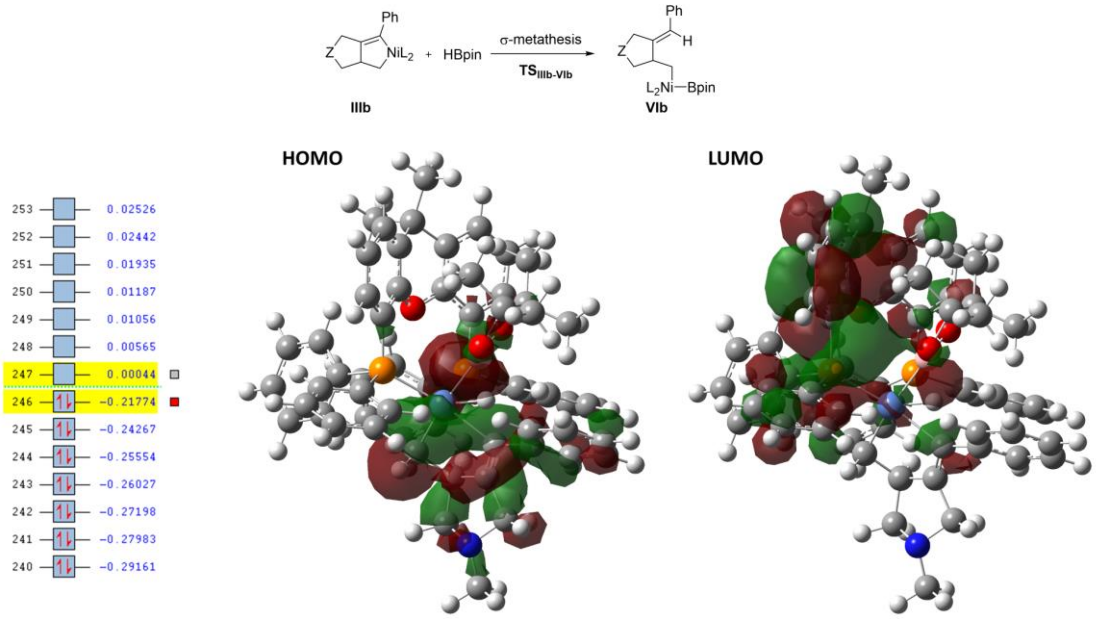
Supplementary Scheme 8. Frontier orbitals for **$TS_{IIIa-VIIa}$**



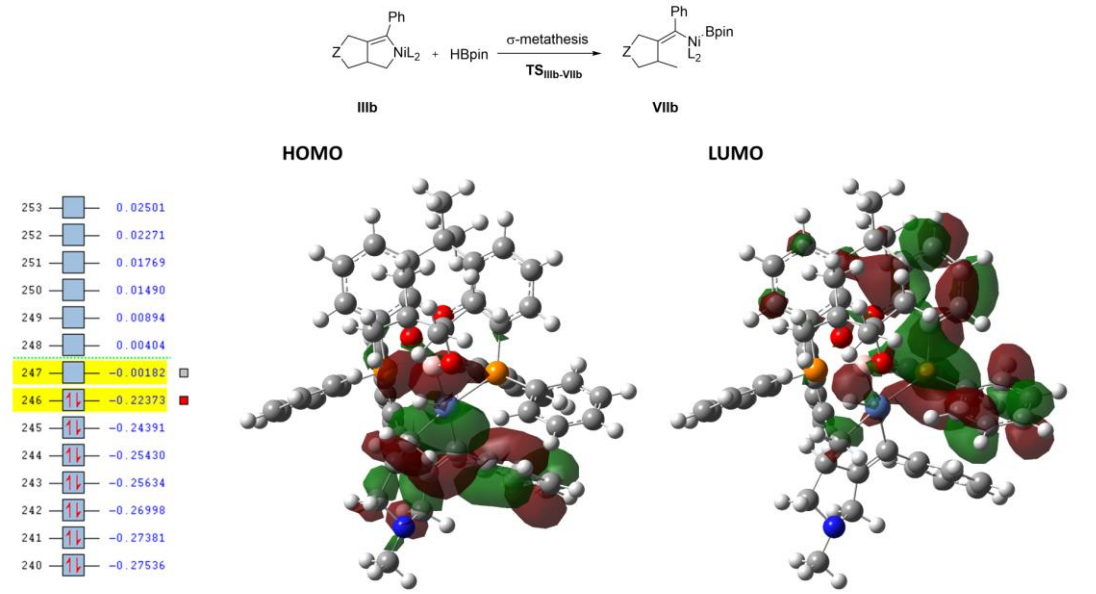
Supplementary Scheme 9. Frontier orbitals for $\mathbf{TS_{IIIb\text{-}IVb}}$



Supplementary Scheme 10. Frontier orbitals for $\mathbf{TS_{IIIb\text{-}Vb}}$



Supplementary Scheme 11. Frontier orbitals for **$TS_{IIIb\text{-}VIb}$**



Supplementary Scheme 12. Frontier orbitals for **$TS_{IIIb\text{-}VIIb}$**

- ***Atomic coordinates and energies for the stationary points***

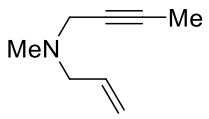
I - L_2Ni^0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.255737	3.923287	-0.722320
2	6	0	3.346322	3.376483	-0.495288
3	6	0	1.039047	1.990060	0.065806
4	6	0	2.207467	4.066099	-0.087140
5	6	0	3.325790	1.990222	-0.617144
6	6	0	2.162740	1.262951	-0.343574
7	6	0	1.032385	3.378642	0.211441
8	1	0	2.240778	5.146966	0.000508
9	1	0	4.218457	1.468928	-0.946796
10	6	0	-0.247045	4.019522	0.740593
11	8	0	-0.111492	1.283846	0.342030
12	6	0	-0.306190	3.787036	2.267975
13	1	0	0.546703	4.271271	2.755087
14	1	0	-0.281331	2.718189	2.503518
15	1	0	-1.231703	4.208002	2.674843
16	6	0	-0.298173	5.521064	0.464187
17	1	0	-0.254745	5.735571	-0.608394
18	1	0	0.535137	6.029096	0.957462
19	1	0	-1.217180	5.952500	0.870599
20	6	0	-1.417282	3.274613	0.106739
21	6	0	-3.514993	1.682026	-0.870095
22	6	0	-2.621808	3.854042	-0.292067
23	6	0	-1.293036	1.891987	-0.022717
24	6	0	-2.315965	1.067274	-0.500972
25	6	0	-3.661593	3.064225	-0.776048
26	1	0	-2.757246	4.928226	-0.220771
27	1	0	-4.595152	3.528324	-1.077756
28	1	0	-4.334860	1.076722	-1.244694
29	15	0	1.995942	-0.558454	-0.631711
30	15	0	-1.955576	-0.735740	-0.667505
31	6	0	-3.597188	-1.368186	-1.213096
32	6	0	-6.055040	-2.265504	-2.207502
33	6	0	-3.763644	-1.613704	-2.579672
34	6	0	-4.673742	-1.585402	-0.346584
35	6	0	-5.895307	-2.034093	-0.841890
36	6	0	-4.988260	-2.053465	-3.077333
37	1	0	-2.922641	-1.460598	-3.252787
38	1	0	-4.554284	-1.405861	0.718632
39	1	0	-6.723775	-2.204107	-0.160814
40	1	0	-5.105941	-2.238659	-4.140647
41	1	0	-7.008039	-2.616892	-2.590995
42	6	0	-1.887790	-1.248321	1.102255
43	6	0	-1.694844	-2.144358	3.749330
44	6	0	-2.433553	-0.495604	2.146532
45	6	0	-1.230719	-2.447001	1.402265
46	6	0	-1.144478	-2.898824	2.715320
47	6	0	-2.333489	-0.940263	3.463771
48	1	0	-2.937321	0.444280	1.933729
49	1	0	-0.763266	-3.013690	0.599650

50	1	0	-0.624158	-3.826350	2.932516
51	1	0	-2.758330	-0.344979	4.266737
52	1	0	-1.615715	-2.488761	4.776264
53	6	0	3.678581	-0.976819	-1.254435
54	6	0	6.189339	-1.562609	-2.342786
55	6	0	4.805059	-1.067860	-0.427591
56	6	0	3.824372	-1.188702	-2.627744
57	6	0	5.074745	-1.475867	-3.172357
58	6	0	6.053079	-1.359950	-0.969296
59	1	0	4.700721	-0.909093	0.642993
60	1	0	2.946356	-1.133603	-3.267620
61	1	0	5.175882	-1.639062	-4.240942
62	1	0	6.921302	-1.428217	-0.320795
63	1	0	7.163841	-1.791473	-2.763507
64	6	0	2.073703	-1.260237	1.073798
65	6	0	2.110210	-2.486245	3.596467
66	6	0	1.809109	-0.518202	2.226694
67	6	0	2.346427	-2.629486	1.199873
68	6	0	2.375573	-3.235794	2.450553
69	6	0	1.821254	-1.130690	3.479196
70	1	0	1.596110	0.544254	2.157075
71	1	0	2.553435	-3.220904	0.310042
72	1	0	2.601751	-4.295084	2.531044
73	1	0	1.604429	-0.541516	4.365281
74	1	0	2.124260	-2.959655	4.573789
75	28	0	0.049317	-1.026762	-1.487275

Zero-point correction=	0.603934
(Hartree/Particle)	
Thermal correction to Energy=	0.640929
Thermal correction to Enthalpy=	0.641874
Thermal correction to Gibbs Free Energy=	0.533631
Sum of electronic and zero-point Energies=	-2431.311589
Sum of electronic and thermal Energies=	-2431.274594
Sum of electronic and thermal Enthalpies=	-2431.273650
Sum of electronic and thermal Free Energies=	-2431.381892

Enyne-Me (A)

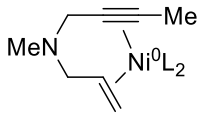


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.374138	-1.126276	0.653708
2	1	0	-0.505147	-2.211524	0.730131
3	1	0	-0.588515	-0.713964	1.657843
4	6	0	1.029563	-0.864444	0.304829
5	6	0	2.194412	-0.693312	0.040914
6	7	0	-1.334542	-0.631614	-0.335746
7	6	0	-1.594653	0.797192	-0.175310
8	1	0	-2.007859	1.019940	0.828710
9	1	0	-2.371020	1.059296	-0.906747

10	6	0	-0.392694	1.662130	-0.421036
11	1	0	0.155692	1.457649	-1.338623
12	6	0	-0.013906	2.646960	0.387820
13	1	0	0.837976	3.278476	0.156571
14	1	0	-0.543610	2.854862	1.314670
15	6	0	-2.584411	-1.369972	-0.224864
16	1	0	-2.405815	-2.432021	-0.413897
17	1	0	-3.290060	-1.002590	-0.975081
18	6	0	3.600748	-0.458677	-0.288872
19	1	0	4.169454	-1.392977	-0.279592
20	1	0	4.061772	0.226315	0.428649
21	1	0	3.696009	-0.016965	-1.285172
22	1	0	-3.056616	-1.266802	0.769630

Zero-point correction= 0.194985
(Hartree/Particle)
Thermal correction to Energy= 0.205941
Thermal correction to Enthalpy= 0.206885
Thermal correction to Gibbs Free Energy= 0.158063
Sum of electronic and zero-point Energies= -366.945134
Sum of electronic and thermal Energies= -366.934178
Sum of electronic and thermal Enthalpies= -366.933234
Sum of electronic and thermal Free Energies= -366.982057

IIa



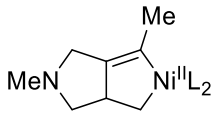
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.303240	-1.679577	-0.463138
2	6	0	0.440048	-3.985162	-2.629693
3	1	0	0.080011	-4.198406	-3.643829
4	1	0	1.529892	-4.128236	-2.641914
5	6	0	0.174838	-2.555988	-2.297693
6	6	0	0.074068	-1.324168	-2.478189
7	7	0	-0.124780	-4.982126	-1.736002
8	6	0	0.286413	-4.765974	-0.350636
9	1	0	1.384977	-4.750784	-0.325234
10	1	0	-0.034566	-5.655200	0.211037
11	6	0	-0.235158	-3.529609	0.350556
12	1	0	-1.319441	-3.467490	0.460722
13	6	0	0.558804	-2.814521	1.239250
14	1	0	0.130598	-2.256320	2.067144
15	1	0	1.606662	-3.094967	1.358513
16	6	0	-1.566953	-5.086448	-1.875836
17	1	0	-1.812142	-5.385079	-2.900346
18	1	0	-2.100813	-4.148466	-1.654564
19	1	0	-1.939904	-5.858421	-1.194683
20	1	0	-1.051231	0.359588	-3.147114
21	1	0	0.074166	-0.300030	-4.348519
22	6	0	-0.060947	-0.089253	-3.281826

23	1	0	0.679837	0.661187	-2.984984
24	1	0	4.465126	2.995977	-2.735194
25	6	0	3.528072	2.792373	-2.227119
26	6	0	1.160464	2.279025	-0.946087
27	6	0	2.417149	3.593909	-2.481344
28	6	0	3.444195	1.723333	-1.338508
29	6	0	2.243086	1.437381	-0.682588
30	6	0	1.205246	3.353233	-1.834437
31	1	0	2.500616	4.409537	-3.191778
32	1	0	4.311329	1.091789	-1.173606
33	6	0	-0.065922	4.181344	-2.001102
34	8	0	-0.020807	1.979658	-0.302084
35	6	0	-0.188891	5.129454	-0.786941
36	1	0	0.663739	5.815799	-0.758354
37	1	0	-0.210401	4.563650	0.150189
38	1	0	-1.112311	5.713677	-0.858969
39	6	0	-0.050476	5.010599	-3.284319
40	1	0	0.038770	4.376658	-4.172409
41	1	0	0.783587	5.717862	-3.273404
42	1	0	-0.966871	5.601820	-3.366514
43	6	0	-1.241564	3.208450	-1.957936
44	6	0	-3.362363	1.397112	-1.566950
45	6	0	-2.409304	3.305437	-2.715560
46	6	0	-1.167480	2.162469	-1.041082
47	6	0	-2.196904	1.249822	-0.811896
48	6	0	-3.458272	2.407585	-2.521976
49	1	0	-2.511498	4.088860	-3.459098
50	1	0	-4.362499	2.502367	-3.114656
51	1	0	-4.187783	0.706845	-1.421750
52	15	0	1.908381	-0.102941	0.280066
53	15	0	-1.829373	-0.119375	0.361171
54	6	0	-3.425442	-1.028594	0.316376
55	6	0	-5.779542	-2.521477	0.068616
56	6	0	-3.560191	-1.979102	-0.703703
57	6	0	-4.480945	-0.833459	1.211101
58	6	0	-5.650643	-1.581106	1.088590
59	6	0	-4.733418	-2.717408	-0.832136
60	1	0	-2.732230	-2.130176	-1.396216
61	1	0	-4.387789	-0.097897	2.005354
62	1	0	-6.464036	-1.426234	1.791082
63	1	0	-4.827308	-3.451462	-1.627244
64	1	0	-6.692368	-3.102333	-0.022186
65	6	0	-1.920040	0.744084	1.986064
66	6	0	-2.002767	1.898281	4.540797
67	6	0	-2.195943	2.105132	2.141358
68	6	0	-1.676724	-0.029164	3.128631
69	6	0	-1.723929	0.540350	4.396284
70	6	0	-2.233782	2.678075	3.411609
71	1	0	-2.395685	2.723492	1.270642
72	1	0	-1.461207	-1.090294	3.024280
73	1	0	-1.528983	-0.073760	5.270349
74	1	0	-2.452354	3.736883	3.516633
75	1	0	-2.033385	2.346405	5.529593
76	6	0	3.553505	-0.927036	0.218682
77	6	0	6.009002	-2.250207	-0.012794
78	6	0	4.660439	-0.500222	0.962131
79	6	0	3.690535	-2.023645	-0.638188

80	6	0	4.913775	-2.681375	-0.756281
81	6	0	5.881028	-1.159619	0.847270
82	1	0	4.562554	0.347829	1.635441
83	1	0	2.825105	-2.358889	-1.207786
84	1	0	5.007748	-3.532201	-1.424417
85	1	0	6.733865	-0.823855	1.429414
86	1	0	6.961765	-2.763759	-0.099154
87	6	0	1.848290	0.478969	2.028091
88	6	0	1.599206	1.188304	4.733558
89	6	0	1.450303	1.768864	2.392594
90	6	0	2.121837	-0.449954	3.041960
91	6	0	2.002173	-0.097811	4.382595
92	6	0	1.324996	2.117971	3.735131
93	1	0	1.234898	2.511822	1.632302
94	1	0	2.448719	-1.452568	2.780542
95	1	0	2.224891	-0.830718	5.152463
96	1	0	1.004312	3.121429	3.998423
97	1	0	1.496481	1.463079	5.779244

Zero-point correction= 0.799787
(Hartree/Particle)
Thermal correction to Energy= 0.848150
Thermal correction to Enthalpy= 0.849095
Thermal correction to Gibbs Free Energy= 0.717796
Sum of electronic and zero-point Energies= -2798.321877
Sum of electronic and thermal Energies= -2798.273514
Sum of electronic and thermal Enthalpies= -2798.272570
Sum of electronic and thermal Free Energies= -2798.403869

IIIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.040173	-4.526720	0.737540
2	6	0	3.595017	-3.635252	0.308030
3	6	0	2.476931	-1.365580	-0.750111
4	6	0	4.371187	-2.785981	-0.482744
5	6	0	2.256892	-3.347101	0.550108
6	6	0	1.665303	-2.195893	0.014554
7	6	0	3.819977	-1.632278	-1.031318
8	1	0	5.413269	-3.028897	-0.663308
9	1	0	1.670043	-4.005852	1.183542
10	6	0	4.543394	-0.636557	-1.935648
11	8	0	1.919630	-0.198952	-1.226740
12	6	0	6.060522	-0.802873	-1.880219
13	1	0	6.345120	-1.801957	-2.222228
14	1	0	6.448433	-0.655828	-0.867054
15	1	0	6.545999	-0.086132	-2.548823
16	6	0	4.066882	-0.853810	-3.389255
17	1	0	2.982220	-0.744000	-3.471569

18	1	0	4.340098	-1.859803	-3.723479
19	1	0	4.541462	-0.121717	-4.050678
20	6	0	4.098832	0.746727	-1.470220
21	6	0	3.070320	3.166526	-0.481022
22	6	0	4.920258	1.861843	-1.332585
23	6	0	2.753102	0.890981	-1.123542
24	6	0	2.215551	2.062875	-0.598287
25	6	0	4.404779	3.068681	-0.858563
26	1	0	5.973707	1.794697	-1.584255
27	1	0	5.056872	3.930216	-0.758926
28	1	0	2.693794	4.097397	-0.069847
29	15	0	-0.128738	-1.769449	0.187736
30	15	0	0.507442	1.994308	0.088164
31	6	0	0.123401	3.792472	0.183667
32	6	0	-0.622928	6.494491	0.159981
33	6	0	0.261922	4.561938	-0.979310
34	6	0	-0.385764	4.395552	1.334669
35	6	0	-0.760628	5.739268	1.319571
36	6	0	-0.103679	5.902275	-0.990863
37	1	0	0.657096	4.108393	-1.885450
38	1	0	-0.493458	3.825228	2.251710
39	1	0	-1.158086	6.192719	2.222285
40	1	0	0.009291	6.482751	-1.901236
41	1	0	-0.916250	7.539548	0.150795
42	6	0	0.828971	1.545985	1.848489
43	6	0	1.139424	0.871995	4.550276
44	6	0	2.106562	1.408653	2.399286
45	6	0	-0.292379	1.309188	2.658954
46	6	0	-0.137895	0.989933	4.004651
47	6	0	2.257571	1.068098	3.743771
48	1	0	2.987534	1.571811	1.785001
49	1	0	-1.292069	1.376280	2.231619
50	1	0	-1.014875	0.812078	4.619120
51	1	0	3.254339	0.964096	4.161340
52	1	0	1.262366	0.616531	5.598498
53	6	0	-0.818243	-2.910412	-1.084760
54	6	0	-1.809015	-4.550387	-3.125829
55	6	0	-0.603093	-4.293427	-1.051689
56	6	0	-1.526629	-2.358436	-2.155952
57	6	0	-2.017486	-3.175775	-3.173458
58	6	0	-1.101013	-5.109158	-2.061966
59	1	0	-0.049616	-4.739056	-0.229453
60	1	0	-1.710075	-1.286187	-2.187577
61	1	0	-2.568071	-2.732658	-3.997512
62	1	0	-0.934052	-6.181104	-2.021124
63	1	0	-2.195794	-5.188399	-3.914537
64	6	0	-0.468990	-2.570518	1.802877
65	6	0	-0.940279	-3.597584	4.364509
66	6	0	0.278804	-2.120167	2.897772
67	6	0	-1.458033	-3.536646	2.005295
68	6	0	-1.690471	-4.047018	3.281750
69	6	0	0.045772	-2.631245	4.169744
70	1	0	1.051761	-1.366931	2.753565
71	1	0	-2.048465	-3.895984	1.167566
72	1	0	-2.460463	-4.798427	3.425920
73	1	0	0.633597	-2.270152	5.008671
74	1	0	-1.122221	-3.998369	5.356956

75	28	0	-1.333397	0.327366	-0.241518
76	1	0	-3.180457	-0.204060	1.276923
77	6	0	-2.929515	-0.712593	0.332459
78	1	0	-2.792377	-1.775731	0.561455
79	6	0	-4.035039	-0.491865	-0.685809
80	6	0	-5.509941	-0.456256	-0.269035
81	7	0	-6.123727	0.295809	-1.365983
82	6	0	-5.216797	1.413894	-1.663518
83	6	0	-3.857939	0.894284	-1.226819
84	1	0	-3.947139	-1.231938	-1.497264
85	1	0	-5.610280	0.077172	0.699298
86	1	0	-5.985334	-1.438871	-0.170006
87	1	0	-5.486445	2.315680	-1.078451
88	1	0	-5.287316	1.686573	-2.725207
89	6	0	-7.479687	0.714205	-1.102915
90	1	0	-7.886402	1.236761	-1.975590
91	1	0	-7.552512	1.395118	-0.232251
92	1	0	-8.108677	-0.160347	-0.905335
93	6	0	-2.675834	1.505838	-1.066608
94	1	0	-1.621947	3.051198	-2.171468
95	6	0	-2.512365	2.929387	-1.541663
96	1	0	-2.391457	3.631463	-0.706560
97	1	0	-3.376137	3.265569	-2.133037

Zero-point correction= 0.803540
(Hartree/Particle)
Thermal correction to Energy= 0.850132
Thermal correction to Enthalpy= 0.851076
Thermal correction to Gibbs Free Energy= 0.724279
Sum of electronic and zero-point Energies= -2798.323704
Sum of electronic and thermal Energies= -2798.277112
Sum of electronic and thermal Enthalpies= -2798.276168
Sum of electronic and thermal Free Energies= -2798.402965

$TS_{IIa\text{-}IIIa}$

Imaginary frequencies = -157.0250 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.387341	1.318522	0.043390
2	1	0	1.796001	2.447671	1.962392
3	6	0	0.849287	2.608012	1.439850
4	1	0	0.046950	2.925160	2.106309
5	6	0	0.964462	3.415191	0.190814
6	6	0	2.210911	4.261372	0.015845
7	7	0	2.191436	4.769555	-1.344404
8	6	0	1.995067	3.608089	-2.195073
9	6	0	1.066927	2.644565	-1.500124
10	1	0	0.080790	4.037648	0.027807
11	1	0	3.113206	3.647950	0.220624
12	1	0	2.207287	5.098522	0.722645
13	1	0	2.963900	3.092686	-2.374470
14	1	0	1.603626	3.906590	-3.175446
15	1	0	3.311463	5.873927	-2.719820
16	6	0	0.530154	1.508088	-1.868631

17	6	0	3.384225	5.510169	-1.690119
18	1	0	3.490195	6.373978	-1.026913
19	1	0	4.300009	4.892527	-1.606963
20	1	0	-0.543820	0.396531	-3.354232
21	6	0	0.461793	0.800152	-3.178759
22	1	0	0.730497	1.436909	-4.032704
23	1	0	1.139840	-0.064243	-3.171305
24	1	0	-4.855774	-0.595311	-3.440295
25	6	0	-3.980246	-0.850273	-2.852297
26	6	0	-1.758406	-1.493319	-1.368900
27	6	0	-3.194575	-1.940966	-3.218221
28	6	0	-3.646939	-0.081255	-1.740933
29	6	0	-2.514885	-0.385714	-0.979710
30	6	0	-2.069620	-2.290283	-2.471631
31	1	0	-3.468449	-2.523021	-4.091970
32	1	0	-4.257240	0.776016	-1.476238
33	6	0	-1.186403	-3.507604	-2.731165
34	8	0	-0.651174	-1.788798	-0.607721
35	6	0	-1.606323	-4.623335	-1.747582
36	1	0	-2.649109	-4.906927	-1.924632
37	1	0	-1.508256	-4.287004	-0.710478
38	1	0	-0.971199	-5.504684	-1.886451
39	6	0	-1.323644	-4.025135	-4.162144
40	1	0	-1.036218	-3.263749	-4.894460
41	1	0	-2.354175	-4.331957	-4.361268
42	1	0	-0.696035	-4.908358	-4.310224
43	6	0	0.246570	-3.102113	-2.400932
44	6	0	2.814548	-2.350188	-1.528011
45	6	0	1.386094	-3.537400	-3.078777
46	6	0	0.438492	-2.271966	-1.298553
47	6	0	1.696280	-1.875750	-0.839255
48	6	0	2.657727	-3.169081	-2.644285
49	1	0	1.287736	-4.173831	-3.951988
50	1	0	3.532590	-3.522848	-3.180284
51	1	0	3.808585	-2.059932	-1.200709
52	15	0	-1.852938	0.695703	0.355424
53	15	0	1.721669	-0.630243	0.507821
54	6	0	3.518082	-0.318154	0.706461
55	6	0	6.235054	0.320484	0.891344
56	6	0	4.039029	0.776263	0.006247
57	6	0	4.369545	-1.087702	1.504374
58	6	0	5.722570	-0.767633	1.595709
59	6	0	5.392014	1.092441	0.093991
60	1	0	3.371214	1.380871	-0.605321
61	1	0	3.972304	-1.933887	2.059279
62	1	0	6.376913	-1.367949	2.220511
63	1	0	5.783690	1.946353	-0.451520
64	1	0	7.289177	0.569013	0.968347
65	6	0	1.289440	-1.616698	1.990456
66	6	0	0.622225	-2.970575	4.343134
67	6	0	1.375890	-3.010699	2.049523
68	6	0	0.850888	-0.907168	3.114236
69	6	0	0.530588	-1.581137	4.288741
70	6	0	1.039211	-3.684410	3.221946
71	1	0	1.706559	-3.570675	1.178147
72	1	0	0.750103	0.175012	3.053581
73	1	0	0.189203	-1.022296	5.154548

74	1	0	1.106133	-4.767683	3.259957
75	1	0	0.360895	-3.497783	5.255895
76	6	0	-3.037049	2.096605	0.301363
77	6	0	-4.769882	4.275921	0.045339
78	6	0	-4.263240	2.105143	0.973698
79	6	0	-2.688556	3.186065	-0.505444
80	6	0	-3.554425	4.269825	-0.635284
81	6	0	-5.123488	3.193025	0.848866
82	1	0	-4.544553	1.259728	1.595391
83	1	0	-1.740226	3.170354	-1.040843
84	1	0	-3.276116	5.110920	-1.262660
85	1	0	-6.072096	3.193716	1.377096
86	1	0	-5.442144	5.123257	-0.049164
87	6	0	-2.302471	-0.164363	1.913371
88	6	0	-2.841674	-1.382134	4.377579
89	6	0	-2.563094	-1.534358	1.982214
90	6	0	-2.294783	0.587065	3.096673
91	6	0	-2.576723	-0.014347	4.317810
92	6	0	-2.825481	-2.139421	3.210431
93	1	0	-2.565664	-2.136286	1.078471
94	1	0	-2.080825	1.652906	3.056175
95	1	0	-2.582539	0.583612	5.224328
96	1	0	-3.020729	-3.206744	3.250691
97	1	0	-3.051870	-1.855452	5.332070

Zero-point correction= 0.800237
(Hartree/Particle)
Thermal correction to Energy= 0.847368
Thermal correction to Enthalpy= 0.848312
Thermal correction to Gibbs Free Energy= 0.718853
Sum of electronic and zero-point Energies= -2798.299450
Sum of electronic and thermal Energies= -2798.252320
Sum of electronic and thermal Enthalpies= -2798.251375
Sum of electronic and thermal Free Energies= -2798.380834

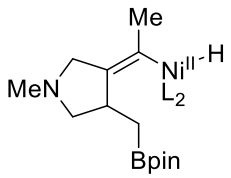
HBPin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.779744	-0.186336	-0.054694
2	8	0	1.062069	1.185607	-0.422129
3	5	0	-0.000417	1.933337	-0.000328
4	1	0	-0.000821	3.120764	-0.000797
5	8	0	-1.062698	1.185284	0.421553
6	6	0	-0.779573	-0.186760	0.054827
7	6	0	-1.345309	-1.109958	1.121393
8	1	0	-2.436214	-1.034405	1.128103
9	1	0	-0.977221	-0.845424	2.114703
10	1	0	-1.075335	-2.149949	0.909143
11	6	0	-1.468714	-0.433904	-1.285203
12	1	0	-1.061674	0.222551	-2.060739
13	1	0	-2.535125	-0.218213	-1.178165
14	1	0	-1.352868	-1.472608	-1.608194
15	6	0	1.469512	-0.432707	1.285152
16	1	0	1.062994	0.224055	2.060651

17	1	0	2.535893	-0.217189	1.177516
18	1	0	1.353676	-1.471265	1.608641
19	6	0	1.345268	-1.110360	-1.120695
20	1	0	0.976932	-0.846796	-2.114153
21	1	0	1.075129	-2.150109	-0.907339
22	1	0	2.436182	-1.035076	-1.127806

Zero-point correction= 0.193501
(Hartree/Particle)
Thermal correction to Energy= 0.202788
Thermal correction to Enthalpy= 0.203732
Thermal correction to Gibbs Free Energy= 0.160716
Sum of electronic and zero-point Energies= -411.491541
Sum of electronic and thermal Energies= -411.482254
Sum of electronic and thermal Enthalpies= -411.481310
Sum of electronic and thermal Free Energies= -411.524326

IVa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.158600	-3.946121	1.035250
2	6	0	3.179848	-3.481080	1.096534
3	6	0	0.706173	-2.308957	1.247694
4	6	0	2.534182	-3.385827	2.328524
5	6	0	2.588021	-2.971156	-0.055861
6	6	0	1.331324	-2.357961	0.002431
7	6	0	1.275622	-2.795853	2.425327
8	1	0	3.022252	-3.771815	3.217574
9	1	0	3.115296	-3.030477	-1.002679
10	6	0	0.456165	-2.665151	3.705286
11	8	0	-0.539436	-1.728100	1.289288
12	6	0	-0.611934	-3.782745	3.713835
13	1	0	-0.126892	-4.764608	3.717080
14	1	0	-1.257387	-3.717123	2.831945
15	1	0	-1.237905	-3.695410	4.608072
16	6	0	1.322199	-2.790961	4.957256
17	1	0	2.102496	-2.023292	4.986033
18	1	0	1.797157	-3.775329	4.996692
19	1	0	0.707633	-2.700084	5.857225
20	6	0	-0.267230	-1.323302	3.635075
21	6	0	-1.808026	1.009500	3.296771
22	6	0	-0.523522	-0.476715	4.713566
23	6	0	-0.778876	-0.944110	2.396134
24	6	0	-1.549911	0.197869	2.189868
25	6	0	-1.285295	0.678062	4.544704
26	1	0	-0.134877	-0.718899	5.697316
27	1	0	-1.480946	1.321876	5.395882
28	1	0	-2.407950	1.906502	3.179600

29	15	0	0.517738	-1.500544	-1.416833
30	15	0	-2.099128	0.524701	0.467446
31	6	0	-3.194114	1.979319	0.708744
32	6	0	-4.771636	4.270798	1.014513
33	6	0	-2.596108	3.241911	0.820933
34	6	0	-4.586899	1.876429	0.755650
35	6	0	-5.371256	3.019114	0.904524
36	6	0	-3.382326	4.379467	0.979828
37	1	0	-1.516579	3.341621	0.764814
38	1	0	-5.064082	0.904829	0.666817
39	1	0	-6.452753	2.927986	0.932977
40	1	0	-2.903994	5.350693	1.066871
41	1	0	-5.384609	5.160142	1.126105
42	6	0	-3.279181	-0.845286	0.157567
43	6	0	-5.109587	-2.862792	-0.468667
44	6	0	-3.843933	-1.622981	1.171935
45	6	0	-3.629686	-1.094287	-1.174284
46	6	0	-4.549440	-2.091763	-1.484526
47	6	0	-4.751789	-2.631711	0.857746
48	1	0	-3.578398	-1.438681	2.209828
49	1	0	-3.171497	-0.511194	-1.971663
50	1	0	-4.810208	-2.279440	-2.521145
51	1	0	-5.184760	-3.233168	1.651452
52	1	0	-5.818901	-3.648698	-0.710771
53	6	0	1.846359	-1.631739	-2.673128
54	6	0	3.991876	-1.769054	-4.458230
55	6	0	2.055585	-2.785194	-3.435368
56	6	0	2.718321	-0.547151	-2.809423
57	6	0	3.790576	-0.620530	-3.695775
58	6	0	3.122824	-2.850685	-4.328306
59	1	0	1.383335	-3.633015	-3.331387
60	1	0	2.560720	0.352168	-2.218218
61	1	0	4.462726	0.226748	-3.796187
62	1	0	3.275665	-3.747310	-4.921343
63	1	0	4.822356	-1.820945	-5.155800
64	6	0	-0.724440	-2.719347	-2.002932
65	6	0	-2.682934	-4.456916	-2.986363
66	6	0	-1.177847	-3.782721	-1.221504
67	6	0	-1.276847	-2.517004	-3.275664
68	6	0	-2.241712	-3.389469	-3.768037
69	6	0	-2.157614	-4.644840	-1.711668
70	1	0	-0.766046	-3.947184	-0.230115
71	1	0	-0.939893	-1.677493	-3.880039
72	1	0	-2.653526	-3.233159	-4.760621
73	1	0	-2.505241	-5.467753	-1.094489
74	1	0	-3.439459	-5.135564	-3.368861
75	6	0	4.156534	1.226272	1.908315
76	8	0	3.058126	2.161936	1.930850
77	5	0	2.521237	2.183218	0.665929
78	8	0	3.330389	1.552776	-0.253770
79	6	0	4.578348	1.247838	0.404304
80	6	0	5.110853	-0.073727	-0.125415
81	1	0	5.389100	0.034031	-1.178152
82	1	0	4.357087	-0.862025	-0.053003
83	1	0	6.000476	-0.379087	0.436890
84	6	0	5.542762	2.386140	0.077801
85	1	0	5.168901	3.337224	0.470367

86	1	0	5.630932	2.474117	-1.008636
87	1	0	6.536963	2.200569	0.495554
88	6	0	3.591941	-0.126794	2.335455
89	1	0	2.845882	-0.484047	1.616641
90	1	0	3.101726	-0.015751	3.307814
91	1	0	4.376529	-0.885112	2.420331
92	6	0	5.228040	1.692431	2.879866
93	1	0	5.524965	2.723993	2.679280
94	1	0	6.112839	1.050268	2.811902
95	1	0	4.843525	1.638606	3.902402
96	6	0	1.117214	2.767620	0.297645
97	1	0	0.804075	3.539919	1.012140
98	1	0	0.414727	1.928462	0.437012
99	6	0	0.999402	3.291255	-1.145896
100	1	0	1.591941	2.641465	-1.801623
101	6	0	-0.431411	3.377203	-1.673241
102	6	0	-0.775300	4.853248	-1.796369
103	1	0	-1.777663	5.102817	-1.424920
104	1	0	-0.716879	5.197225	-2.851477
105	7	0	0.248431	5.509362	-0.982529
106	6	0	1.466343	4.749050	-1.248178
107	1	0	2.250861	5.013900	-0.527510
108	1	0	1.850880	4.962145	-2.265757
109	6	0	0.382918	6.920779	-1.261076
110	1	0	-0.561544	7.433649	-1.051532
111	1	0	0.653266	7.117088	-2.316696
112	1	0	1.158223	7.355812	-0.621872
113	6	0	-1.207113	2.323729	-1.948319
114	6	0	-2.577972	2.488020	-2.553439
115	1	0	-2.914781	3.533599	-2.584366
116	1	0	-3.341087	1.917430	-2.007158
117	1	0	-2.581292	2.105668	-3.582414
118	28	0	-0.585393	0.589409	-1.421109
119	1	0	-0.014911	0.732447	-2.801423

Zero-point correction= 0.996051
(Hartree/Particle)
Thermal correction to Energy= 1.053602
Thermal correction to Enthalpy= 1.054546
Thermal correction to Gibbs Free Energy= 0.904755
Sum of electronic and zero-point Energies= -3209.869292
Sum of electronic and thermal Energies= -3209.811741
Sum of electronic and thermal Enthalpies= -3209.810797
Sum of electronic and thermal Free Energies= -3209.960588

$TS_{IIIa\text{-}IVa}$

imaginary frequencies = -267.9386 cm^{-1}

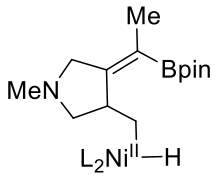
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.655619	0.378319	-0.256222
2	1	0	3.157734	-0.898808	1.004147
3	6	0	2.274335	-0.259417	1.047966
4	1	0	1.606423	-0.829545	1.706129
5	6	0	2.636881	1.104106	1.674561

6	6	0	4.090856	1.309649	2.122893
7	7	0	4.282309	2.756374	2.030437
8	6	0	3.674723	3.133936	0.750271
9	6	0	2.513385	2.179216	0.620286
10	1	0	1.983034	1.309705	2.538521
11	1	0	4.760380	0.779825	1.418609
12	1	0	4.302527	0.955692	3.138512
13	1	0	4.372255	2.958155	-0.097259
14	1	0	3.403040	4.197360	0.744232
15	1	0	5.751322	4.243005	2.059239
16	6	0	1.694528	1.994543	-0.415651
17	6	0	5.667540	3.153883	2.136390
18	1	0	6.070720	2.846709	3.107043
19	1	0	6.295100	2.703667	1.342517
20	1	0	1.216614	2.360463	-2.502726
21	6	0	1.885285	2.725904	-1.717498
22	1	0	1.732013	3.810335	-1.632082
23	1	0	2.915136	2.545063	-2.054282
24	1	0	1.750547	-0.444794	-1.703453
25	5	0	2.761392	-0.579109	-1.003572
26	8	0	3.845530	0.337736	-1.164022
27	6	0	4.909300	-0.382533	-1.778235
28	6	0	4.702697	-1.830658	-1.229078
29	8	0	3.287662	-1.898481	-1.078999
30	6	0	6.234439	0.264090	-1.399193
31	1	0	6.279316	1.277036	-1.812838
32	1	0	7.077761	-0.308507	-1.802646
33	1	0	6.346270	0.336790	-0.314447
34	6	0	4.711808	-0.304408	-3.295803
35	1	0	4.664692	0.749816	-3.585902
36	1	0	3.769733	-0.780732	-3.586336
37	1	0	5.530667	-0.781623	-3.844032
38	6	0	5.376830	-2.058962	0.126331
39	1	0	5.178395	-1.240610	0.823149
40	1	0	6.462474	-2.162726	0.019842
41	1	0	4.975482	-2.982376	0.556494
42	6	0	5.143660	-2.932672	-2.187251
43	1	0	4.550755	-2.915313	-3.104703
44	1	0	5.004641	-3.908983	-1.712476
45	1	0	6.203526	-2.823069	-2.445846
46	1	0	-5.668166	3.203533	-2.471761
47	6	0	-5.084325	2.407318	-2.021920
48	6	0	-3.617230	0.402483	-0.856432
49	6	0	-5.613265	1.121302	-1.939702
50	6	0	-3.812419	2.680041	-1.531210
51	6	0	-3.033899	1.663303	-0.965726
52	6	0	-4.892040	0.094190	-1.335576
53	1	0	-6.604690	0.928718	-2.335778
54	1	0	-3.418252	3.686779	-1.603761
55	6	0	-5.425088	-1.310276	-1.077863
56	8	0	-2.879009	-0.556898	-0.209593
57	6	0	-5.949435	-1.359156	0.375911
58	1	0	-6.775950	-0.651505	0.499721
59	1	0	-5.158591	-1.098663	1.086728
60	1	0	-6.306933	-2.366859	0.611556
61	6	0	-6.559592	-1.682098	-2.032117
62	1	0	-6.231998	-1.659347	-3.076213

63	1	0	-7.401456	-0.994771	-1.913245
64	1	0	-6.937523	-2.682512	-1.804672
65	6	0	-4.246515	-2.271337	-1.181669
66	6	0	-2.006627	-3.965974	-1.053795
67	6	0	-4.319241	-3.581487	-1.651399
68	6	0	-3.016513	-1.840440	-0.685986
69	6	0	-1.882322	-2.645600	-0.611691
70	6	0	-3.210555	-4.421677	-1.584089
71	1	0	-5.250035	-3.961360	-2.059074
72	1	0	-3.287719	-5.444374	-1.938254
73	1	0	-1.159397	-4.639734	-0.992115
74	15	0	-1.313331	1.905958	-0.329301
75	15	0	-0.389374	-1.887366	0.173299
76	6	0	0.835963	-3.234103	-0.022611
77	6	0	2.784327	-5.202976	-0.406624
78	6	0	1.104165	-3.727850	-1.304300
79	6	0	1.571445	-3.718264	1.060735
80	6	0	2.547611	-4.693108	0.866546
81	6	0	2.057455	-4.720467	-1.492412
82	1	0	0.565573	-3.331774	-2.162518
83	1	0	1.386059	-3.336495	2.060620
84	1	0	3.116446	-5.059120	1.716226
85	1	0	2.249974	-5.101126	-2.491016
86	1	0	3.537268	-5.971865	-0.553817
87	6	0	-0.901663	-2.038069	1.938234
88	6	0	-1.705910	-2.240431	4.608941
89	6	0	-1.406854	-3.245974	2.436712
90	6	0	-0.807522	-0.935907	2.788716
91	6	0	-1.208120	-1.036864	4.121228
92	6	0	-1.804559	-3.347214	3.764379
93	1	0	-1.483945	-4.110526	1.781538
94	1	0	-0.416477	0.006590	2.415760
95	1	0	-1.129566	-0.169159	4.768518
96	1	0	-2.191947	-4.288395	4.142157
97	1	0	-2.018004	-2.320313	5.645856
98	6	0	-0.979312	3.571007	-1.035066
99	6	0	-0.367910	6.014032	-2.260124
100	6	0	-0.998572	3.694132	-2.430629
101	6	0	-0.664171	4.687525	-0.261195
102	6	0	-0.352087	5.901474	-0.873606
103	6	0	-0.703149	4.907085	-3.039799
104	1	0	-1.245931	2.831297	-3.045831
105	1	0	-0.658020	4.622221	0.821399
106	1	0	-0.100135	6.760824	-0.260096
107	1	0	-0.721988	4.985953	-4.122203
108	1	0	-0.125356	6.960244	-2.733731
109	6	0	-1.625999	2.213849	1.459794
110	6	0	-1.954305	2.542368	4.224070
111	6	0	-2.873491	2.003976	2.053935
112	6	0	-0.541107	2.585144	2.267264
113	6	0	-0.706832	2.755675	3.638467
114	6	0	-3.032559	2.163830	3.429625
115	1	0	-3.729404	1.715452	1.451882
116	1	0	0.434334	2.734697	1.812116
117	1	0	0.143602	3.047876	4.247039
118	1	0	-4.006126	1.992863	3.878502
119	1	0	-2.083821	2.667756	5.294998

```
 ---------------------------------------------------------------------
 Zero-point correction=                           0.998184
(Hartree/Particle)
 Thermal correction to Energy=                    1.054481
 Thermal correction to Enthalpy=                  1.055425
 Thermal correction to Gibbs Free Energy=         0.910540
 Sum of electronic and zero-point Energies=          -3209.794136
 Sum of electronic and thermal Energies=             -3209.737839
 Sum of electronic and thermal Enthalpies=           -3209.736895
 Sum of electronic and thermal Free Energies=        -3209.881780
```

Va



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.729174	2.701214	-0.862700
2	6	0	-5.970391	1.945740	-0.687215
3	6	0	-4.052606	0.037327	-0.249019
4	6	0	-6.285150	0.598632	-0.854885
5	6	0	-4.689680	2.332975	-0.303834
6	6	0	-3.694777	1.374513	-0.082493
7	6	0	-5.325912	-0.387020	-0.629839
8	1	0	-7.287842	0.320513	-1.162249
9	1	0	-4.457034	3.386998	-0.196267
10	6	0	-5.563478	-1.891654	-0.718243
11	8	0	-3.066458	-0.897907	-0.026329
12	6	0	-5.738328	-2.438196	0.717245
13	1	0	-6.616343	-1.982636	1.186817
14	1	0	-4.859765	-2.215962	1.331539
15	1	0	-5.875538	-3.524219	0.689779
16	6	0	-6.805812	-2.233276	-1.539093
17	1	0	-6.724042	-1.863670	-2.566142
18	1	0	-7.698239	-1.798806	-1.080105
19	1	0	-6.959008	-3.315666	-1.566694
20	6	0	-4.296640	-2.505803	-1.305853
21	6	0	-1.827730	-3.571449	-2.136498
22	6	0	-4.248745	-3.590071	-2.181311
23	6	0	-3.079408	-1.972532	-0.886237
24	6	0	-1.837757	-2.465266	-1.282985
25	6	0	-3.025943	-4.120670	-2.587417
26	1	0	-5.169323	-4.033226	-2.546711
27	1	0	-3.006358	-4.973011	-3.258522
28	1	0	-0.882984	-3.996593	-2.459336
29	15	0	-1.922930	1.757951	0.264176
30	15	0	-0.352490	-1.581121	-0.648704
31	6	0	0.987327	-2.627226	-1.335683
32	6	0	3.013708	-4.154657	-2.515266
33	6	0	1.291244	-2.477767	-2.695312
34	6	0	1.710172	-3.546712	-0.573766

35	6	0	2.723532	-4.302767	-1.162781
36	6	0	2.291354	-3.242513	-3.284337
37	1	0	0.739564	-1.755774	-3.294573
38	1	0	1.489174	-3.672456	0.482660
39	1	0	3.285931	-5.008975	-0.559314
40	1	0	2.515983	-3.117992	-4.338962
41	1	0	3.804133	-4.743188	-2.970520
42	6	0	-0.379736	-2.031970	1.131294
43	6	0	-0.314318	-2.632010	3.862383
44	6	0	-1.096816	-3.122983	1.631464
45	6	0	0.365928	-1.240570	2.011981
46	6	0	0.403275	-1.544620	3.370708
47	6	0	-1.065955	-3.418425	2.992097
48	1	0	-1.681100	-3.745208	0.958647
49	1	0	0.908737	-0.376287	1.630114
50	1	0	0.975592	-0.916734	4.046767
51	1	0	-1.628623	-4.266238	3.371327
52	1	0	-0.294539	-2.862048	4.923442
53	6	0	-1.939612	3.586310	0.138436
54	6	0	-2.000010	6.359006	-0.201845
55	6	0	-2.454909	4.407807	1.145391
56	6	0	-1.448809	4.164060	-1.035650
57	6	0	-1.485411	5.545050	-1.208900
58	6	0	-2.481633	5.790314	0.975883
59	1	0	-2.832829	3.965356	2.063945
60	1	0	-1.015053	3.524817	-1.801120
61	1	0	-1.099107	5.984940	-2.123126
62	1	0	-2.876422	6.423758	1.764267
63	1	0	-2.019075	7.436770	-0.331277
64	6	0	-1.751935	1.470388	2.070924
65	6	0	-1.300262	0.998675	4.790866
66	6	0	-2.629802	0.666939	2.801072
67	6	0	-0.633201	2.023619	2.710117
68	6	0	-0.415740	1.795628	4.064802
69	6	0	-2.400564	0.430707	4.155840
70	1	0	-3.497878	0.225676	2.319987
71	1	0	0.063152	2.633783	2.139814
72	1	0	0.447841	2.238643	4.552199
73	1	0	-3.087404	-0.197599	4.714828
74	1	0	-1.127496	0.816379	5.847436
75	6	0	4.159611	1.377113	-2.042024
76	6	0	2.820202	1.765059	-1.414633
77	6	0	2.195164	2.673374	-2.488009
78	7	0	3.307526	3.119900	-3.317986
79	6	0	4.172255	1.952700	-3.441089
80	1	0	2.995603	2.333644	-0.496358
81	1	0	1.469943	2.080590	-3.086969
82	1	0	1.652706	3.525741	-2.065121
83	1	0	5.166018	2.241669	-3.798882
84	1	0	3.755175	1.215670	-4.163304
85	6	0	2.893345	3.661102	-4.590584
86	1	0	2.331307	2.922856	-5.196808
87	1	0	3.767516	3.981502	-5.166725
88	1	0	2.249659	4.532267	-4.431437
89	6	0	5.128375	0.644951	-1.470285
90	6	0	1.929990	0.555991	-1.110279
91	1	0	2.391839	-0.052207	-0.316645

92	1	0	1.911329	-0.078848	-2.009929
93	28	0	0.050596	0.813350	-0.630123
94	1	0	0.522366	2.194608	-0.297307
95	6	0	6.365906	0.195698	-2.217836
96	1	0	6.472816	-0.892816	-2.148244
97	1	0	7.277813	0.623964	-1.783223
98	1	0	6.341109	0.462524	-3.277709
99	5	0	5.032531	0.189526	0.012377
100	8	0	5.664723	-0.946056	0.477119
101	8	0	4.402061	0.877804	1.026401
102	6	0	5.209117	-1.161270	1.827914
103	6	0	4.811972	0.281379	2.270379
104	6	0	4.007715	-2.102988	1.750694
105	1	0	3.621067	-2.350728	2.744995
106	1	0	4.314707	-3.026326	1.250529
107	1	0	3.197035	-1.657116	1.163129
108	6	0	6.328862	-1.793792	2.638153
109	1	0	6.032988	-1.892700	3.688370
110	1	0	7.243532	-1.199882	2.584697
111	1	0	6.544290	-2.792502	2.247564
112	6	0	3.655687	0.353513	3.253523
113	1	0	3.898483	-0.180896	4.178962
114	1	0	3.447216	1.398929	3.499972
115	6	0	6.001830	1.089629	2.785923
116	1	0	6.332725	0.735962	3.767304
117	1	0	5.703513	2.137821	2.873228
118	1	0	6.843782	1.029702	2.088966
119	1	0	2.754171	-0.081849	2.819506

Zero-point correction=	0.996023
(Hartree/Particle)	
Thermal correction to Energy=	1.053943
Thermal correction to Enthalpy=	1.054887
Thermal correction to Gibbs Free Energy=	0.901459
Sum of electronic and zero-point Energies=	-3209.854235
Sum of electronic and thermal Energies=	-3209.796315
Sum of electronic and thermal Enthalpies=	-3209.795371
Sum of electronic and thermal Free Energies=	-3209.948799

$TS_{IIIa\text{-}Va}$

imaginary frequencies = -134.8575 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.860966	-0.236654	0.136907
2	1	0	2.481484	-1.911313	0.862403
3	6	0	1.848021	-1.286624	1.500326
4	1	0	1.291625	-1.931319	2.190866
5	6	0	2.651435	-0.240463	2.234468
6	6	0	3.941171	-0.567210	2.992298
7	7	0	4.504923	0.769075	3.196666
8	6	0	4.290008	1.516043	1.950516
9	6	0	3.134044	0.802762	1.274617
10	1	0	2.000771	0.271012	2.967532
11	1	0	4.595148	-1.204720	2.364348

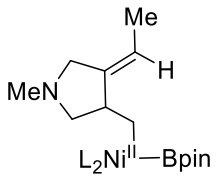
12	1	0	3.788480	-1.067519	3.954881
13	1	0	5.176478	1.471728	1.285225
14	1	0	4.107704	2.580198	2.160645
15	1	0	6.220632	1.792260	3.810488
16	6	0	2.649514	1.011562	0.032449
17	6	0	5.881610	0.765940	3.634291
18	1	0	5.970300	0.211265	4.574029
19	1	0	6.560937	0.302835	2.893095
20	1	0	2.694724	2.546227	-1.544737
21	6	0	3.183496	2.291762	-0.607520
22	1	0	3.074270	3.143475	0.076754
23	1	0	4.255466	2.186231	-0.833246
24	1	0	1.049028	-0.054499	-1.739533
25	5	0	2.294760	-0.142815	-1.602550
26	8	0	3.041003	0.516477	-2.610754
27	6	0	3.920341	-0.432488	-3.214742
28	6	0	4.082580	-1.504927	-2.095300
29	8	0	2.799501	-1.468121	-1.470324
30	6	0	5.211891	0.267558	-3.614610
31	1	0	5.007566	0.993512	-4.407482
32	1	0	5.944638	-0.454585	-3.992239
33	1	0	5.647590	0.802681	-2.767723
34	6	0	3.219090	-0.989894	-4.455197
35	1	0	2.942871	-0.154816	-5.105535
36	1	0	2.304933	-1.521641	-4.172788
37	1	0	3.865013	-1.671115	-5.018956
38	6	0	5.146779	-1.118173	-1.064868
39	1	0	5.011107	-0.086232	-0.727623
40	1	0	6.157255	-1.231162	-1.471818
41	1	0	5.044341	-1.773090	-0.193367
42	6	0	4.335029	-2.921738	-2.592017
43	1	0	3.505410	-3.275930	-3.208908
44	1	0	4.436624	-3.594004	-1.733505
45	1	0	5.259421	-2.973967	-3.178109
46	1	0	-4.429966	4.331216	-2.498760
47	6	0	-4.089125	3.406074	-2.045517
48	6	0	-3.247200	1.072627	-0.872200
49	6	0	-4.862296	2.251134	-2.164973
50	6	0	-2.870789	3.372426	-1.376182
51	6	0	-2.413141	2.184920	-0.792540
52	6	0	-4.453441	1.057582	-1.575607
53	1	0	-5.791116	2.288520	-2.724799
54	1	0	-2.252673	4.264025	-1.332416
55	6	0	-5.229265	-0.255581	-1.610921
56	8	0	-2.816895	-0.069297	-0.240229
57	6	0	-5.990479	-0.407635	-0.273855
58	1	0	-6.709384	0.410019	-0.156873
59	1	0	-5.300026	-0.388288	0.575481
60	1	0	-6.532434	-1.359180	-0.258277
61	6	0	-6.228076	-0.303546	-2.765838
62	1	0	-5.730055	-0.193290	-3.734230
63	1	0	-6.971929	0.491196	-2.661519
64	1	0	-6.774892	-1.250576	-2.757890
65	6	0	-4.201140	-1.381141	-1.689707
66	6	0	-2.286347	-3.435047	-1.459646
67	6	0	-4.351987	-2.577892	-2.389843
68	6	0	-3.047954	-1.238977	-0.921038

69	6	0	-2.092767	-2.240583	-0.762018
70	6	0	-3.398981	-3.589806	-2.283710
71	1	0	-5.223790	-2.732990	-3.017170
72	1	0	-3.534871	-4.515729	-2.832706
73	1	0	-1.567983	-4.242449	-1.359081
74	15	0	-0.725877	1.965400	-0.075310
75	15	0	-0.716723	-1.909757	0.416047
76	6	0	-0.003393	-3.592001	0.550054
77	6	0	1.060608	-6.174327	0.554830
78	6	0	1.034644	-3.924796	-0.328039
79	6	0	-0.496008	-4.553054	1.436105
80	6	0	0.038661	-5.839444	1.439595
81	6	0	1.557227	-5.215942	-0.326840
82	1	0	1.454011	-3.167892	-0.989208
83	1	0	-1.291372	-4.300848	2.131025
84	1	0	-0.345028	-6.578915	2.135659
85	1	0	2.362653	-5.468798	-1.010030
86	1	0	1.474276	-7.178199	0.557519
87	6	0	-1.655125	-1.616222	1.967874
88	6	0	-3.092959	-1.007514	4.288112
89	6	0	-2.879992	-2.243657	2.225128
90	6	0	-1.164218	-0.676335	2.877984
91	6	0	-1.880963	-0.372506	4.033516
92	6	0	-3.591257	-1.944914	3.383480
93	1	0	-3.286204	-2.955963	1.510660
94	1	0	-0.226775	-0.166016	2.675043
95	1	0	-1.492076	0.372471	4.720839
96	1	0	-4.539819	-2.437165	3.575012
97	1	0	-3.655272	-0.768174	5.185425
98	6	0	0.110923	3.359677	-0.926261
99	6	0	1.385022	5.367467	-2.399576
100	6	0	0.353087	3.190879	-2.295888
101	6	0	0.506850	4.543765	-0.303824
102	6	0	1.149249	5.540241	-1.038964
103	6	0	0.977947	4.191790	-3.030488
104	1	0	0.064036	2.262722	-2.785097
105	1	0	0.320065	4.692455	0.755801
106	1	0	1.461335	6.455147	-0.544236
107	1	0	1.164216	4.046683	-4.089943
108	1	0	1.885719	6.145421	-2.967592
109	6	0	-0.922230	2.557135	1.652090
110	6	0	-1.094259	3.295502	4.347909
111	6	0	-2.152900	2.908247	2.209643
112	6	0	0.224765	2.574417	2.459552
113	6	0	0.139853	2.946614	3.797369
114	6	0	-2.237196	3.272385	3.553231
115	1	0	-3.050538	2.895258	1.598463
116	1	0	1.184778	2.289524	2.030437
117	1	0	1.037064	2.956419	4.409186
118	1	0	-3.200445	3.539999	3.977133
119	1	0	-1.162637	3.581199	5.393282

Zero-point correction= 0.997986
(Hartree/Particle)
Thermal correction to Energy= 1.054557
Thermal correction to Enthalpy= 1.055501
Thermal correction to Gibbs Free Energy= 0.907461

Sum of electronic and zero-point Energies= -3209.815106
Sum of electronic and thermal Energies= -3209.758535
Sum of electronic and thermal Enthalpies= -3209.757591
Sum of electronic and thermal Free Energies= -3209.905630

VIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	2.778030	-4.054823	0.773090
3	6	0	1.495828	-3.343536	0.312441
4	6	0	1.908033	-2.934868	-1.099515
5	6	0	3.423323	-2.904958	-1.152356
6	7	0	3.833154	-3.208861	0.217390
7	1	0	2.836812	-5.083422	0.360233
8	1	0	3.836064	-1.940247	-1.478476
9	1	0	3.785393	-3.675816	-1.862814
10	6	0	5.158445	-3.773543	0.311966
11	1	0	5.893597	-3.069727	-0.092880
12	1	0	5.405743	-3.961830	1.361612
13	6	0	1.082619	-2.733225	-2.130303
14	6	0	1.497745	-2.375559	-3.529491
15	1	0	1.250435	-3.183380	-4.229507
16	1	0	2.575379	-2.191795	-3.595864
17	1	0	0.969893	-1.475239	-3.865865
18	28	0	0.312795	-0.789303	-0.082912
19	5	0	-0.452753	0.479727	-1.530698
20	8	0	-1.170067	1.638869	-1.281510
21	6	0	-1.748320	2.138803	-2.493751
22	6	0	-0.820804	1.504383	-3.574491
23	8	0	-0.358373	0.304654	-2.916733
24	1	0	0.650819	-4.041571	0.260132
25	6	0	1.132060	-2.131330	1.185878
26	1	0	0.013790	-2.874664	-1.961119
27	1	0	2.052135	-1.745621	1.632381
28	1	0	0.490706	-2.452795	2.014686
29	6	0	-1.737046	3.659671	-2.431477
30	1	0	-2.391298	3.983665	-1.614842
31	1	0	-2.105320	4.097072	-3.366330
32	1	0	-0.733783	4.041320	-2.226752
33	6	0	-3.187416	1.628205	-2.547733
34	1	0	-3.710206	1.964489	-1.646235
35	1	0	-3.215113	0.533214	-2.560579
36	1	0	-3.719210	2.006734	-3.427053
37	6	0	0.412374	2.357804	-3.862474
38	1	0	0.152865	3.268324	-4.412095
39	1	0	1.116697	1.774332	-4.463982
40	1	0	0.915440	2.636616	-2.929434

41	6	0	-1.516615	1.116288	-4.869527
42	1	0	-2.309893	0.386411	-4.688568
43	1	0	-0.791435	0.672252	-5.558477
44	1	0	-1.953628	1.996771	-5.353742
45	1	0	5.253349	-4.726956	-0.242849
46	1	0	1.517728	5.781755	0.127608
47	6	0	1.041643	4.852215	0.422412
48	6	0	-0.188160	2.481149	1.137070
49	6	0	-0.205485	4.872820	1.040011
50	6	0	1.685893	3.639298	0.199733
51	6	0	1.082724	2.430121	0.552753
52	6	0	-0.831340	3.687555	1.421410
53	1	0	-0.690839	5.824880	1.226975
54	1	0	2.664010	3.630315	-0.271342
55	6	0	-2.148645	3.608004	2.179678
56	8	0	-0.822028	1.293250	1.441483
57	6	0	-1.835565	3.300580	3.662332
58	1	0	-1.246997	4.115385	4.097318
59	1	0	-1.266154	2.371201	3.759182
60	1	0	-2.767543	3.196929	4.228109
61	6	0	-2.939100	4.913513	2.105586
62	1	0	-3.189155	5.176107	1.072231
63	1	0	-2.363286	5.732427	2.545696
64	1	0	-3.865556	4.834594	2.680947
65	6	0	-2.919793	2.429063	1.600535
66	6	0	-4.201627	0.119397	0.690781
67	6	0	-4.301257	2.408716	1.425048
68	6	0	-2.191483	1.276555	1.284241
69	6	0	-2.809508	0.106395	0.823252
70	6	0	-4.944076	1.258018	0.978142
71	1	0	-4.886752	3.293758	1.650086
72	1	0	-6.021802	1.249469	0.852627
73	1	0	-4.711665	-0.766791	0.328256
74	15	0	1.891821	0.797684	0.297277
75	15	0	-1.822301	-1.386520	0.363007
76	6	0	-2.888500	-2.230440	-0.884379
77	6	0	-4.472039	-3.460486	-2.848271
78	6	0	-2.583752	-2.080390	-2.242534
79	6	0	-3.991442	-3.017675	-0.524254
80	6	0	-4.777648	-3.625667	-1.498486
81	6	0	-3.374833	-2.687916	-3.217066
82	1	0	-1.727776	-1.483029	-2.545494
83	1	0	-4.233739	-3.162104	0.524905
84	1	0	-5.629019	-4.230575	-1.202199
85	1	0	-3.123817	-2.560379	-4.265932
86	1	0	-5.084388	-3.937362	-3.607485
87	6	0	-2.065641	-2.456653	1.840451
88	6	0	-2.141045	-4.102509	4.107598
89	6	0	-2.286144	-1.909049	3.105659
90	6	0	-1.875524	-3.839147	1.723789
91	6	0	-1.918695	-4.657112	2.847866
92	6	0	-2.323269	-2.728632	4.232872
93	1	0	-2.426347	-0.837192	3.217679
94	1	0	-1.700546	-4.280592	0.745181
95	1	0	-1.774212	-5.727839	2.740355
96	1	0	-2.494994	-2.288428	5.210412
97	1	0	-2.169285	-4.739078	4.986378

98	6	0	3.159066	1.091678	-0.999393
99	6	0	5.051294	1.408689	-3.038179
100	6	0	2.918534	0.572322	-2.275040
101	6	0	4.365993	1.758234	-0.749603
102	6	0	5.302881	1.921327	-1.765516
103	6	0	3.860961	0.733012	-3.290703
104	1	0	1.990231	0.041236	-2.469544
105	1	0	4.577103	2.137839	0.246884
106	1	0	6.234324	2.440571	-1.561980
107	1	0	3.663469	0.320340	-4.276257
108	1	0	5.787844	1.530284	-3.826575
109	6	0	2.948278	0.707295	1.805715
110	6	0	4.565363	0.447946	4.079426
111	6	0	2.733346	1.516618	2.923471
112	6	0	3.976313	-0.245475	1.841954
113	6	0	4.780271	-0.369095	2.969871
114	6	0	3.537883	1.385205	4.055179
115	1	0	1.940483	2.259062	2.918208
116	1	0	4.126653	-0.921556	1.001388
117	1	0	5.571537	-1.113149	2.984659
118	1	0	3.359677	2.022907	4.915877
119	1	0	5.192951	0.349885	4.960161

Zero-point correction= 1.000377
(Hartree/Particle)
Thermal correction to Energy= 1.057551
Thermal correction to Enthalpy= 1.058496
Thermal correction to Gibbs Free Energy= 0.911266
Sum of electronic and zero-point Energies= -3209.847185
Sum of electronic and thermal Energies= -3209.790011
Sum of electronic and thermal Enthalpies= -3209.789067
Sum of electronic and thermal Free Energies= -3209.936296

$TS_{IIIa\text{-}VIa}$

Imaginary frequency: -1142.1454

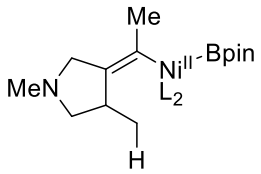
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.351273	1.069590	1.329151
2	6	0	5.250138	0.607682	0.340671
3	6	0	3.778282	0.333400	-0.047385
4	6	0	3.710832	0.780204	-1.488273
5	6	0	5.127768	1.048618	-1.938976
6	7	0	5.748624	1.510687	-0.698802
7	1	0	5.832594	-0.335853	0.342527
8	1	0	5.227075	1.804293	-2.723847
9	1	0	5.605285	0.111803	-2.302823
10	6	0	7.190740	1.566253	-0.763765
11	1	0	7.504259	2.259260	-1.551337
12	1	0	7.590948	1.927356	0.188876
13	6	0	2.549644	1.058593	-2.089687
14	6	0	2.452938	1.632602	-3.483599
15	1	0	1.921277	0.948467	-4.159951
16	1	0	3.433251	1.842228	-3.923169
17	1	0	1.879487	2.569501	-3.474507

18	28	0	1.106860	0.836643	-0.490334
19	5	0	-0.388218	0.816765	-2.099919
20	8	0	-0.772460	-0.134903	-3.013237
21	6	0	-2.013850	0.289908	-3.623405
22	6	0	-2.029789	1.826693	-3.329077
23	8	0	-1.195782	1.932163	-2.151299
24	1	0	3.598864	-0.752442	-0.000107
25	6	0	2.666752	1.068042	0.709245
26	1	0	1.089570	0.779923	-2.048343
27	1	0	2.911986	2.141667	0.742082
28	1	0	2.569632	0.710407	1.741153
29	6	0	-3.136675	-0.464842	-2.923140
30	1	0	-2.924268	-1.536877	-2.972059
31	1	0	-4.106115	-0.271306	-3.395120
32	1	0	-3.198776	-0.176955	-1.869982
33	6	0	-1.976769	-0.077222	-5.099088
34	1	0	-1.967213	-1.166144	-5.201366
35	1	0	-1.085010	0.320020	-5.588337
36	1	0	-2.863957	0.307899	-5.613488
37	6	0	-3.401225	2.399843	-3.010582
38	1	0	-4.077502	2.274481	-3.863545
39	1	0	-3.307410	3.469531	-2.800289
40	1	0	-3.840512	1.919169	-2.133396
41	6	0	-1.347763	2.653562	-4.417594
42	1	0	-0.355488	2.252431	-4.646708
43	1	0	-1.226060	3.678606	-4.055779
44	1	0	-1.939490	2.675187	-5.337885
45	1	0	7.640792	0.576309	-0.973732
46	1	0	-5.229740	2.996872	0.598054
47	6	0	-4.519190	2.179368	0.665732
48	6	0	-2.721028	0.114006	0.806508
49	6	0	-4.966455	0.864242	0.549259
50	6	0	-3.168206	2.454950	0.859727
51	6	0	-2.236218	1.416322	0.935769
52	6	0	-4.069460	-0.199994	0.629090
53	1	0	-6.023200	0.672296	0.395981
54	1	0	-2.834702	3.484893	0.928106
55	6	0	-4.448776	-1.678146	0.583555
56	8	0	-1.790792	-0.898739	0.853854
57	6	0	-4.463875	-2.213354	2.033668
58	1	0	-5.210597	-1.675681	2.627338
59	1	0	-3.484778	-2.085214	2.507903
60	1	0	-4.710085	-3.280418	2.036253
61	6	0	-5.821908	-1.898381	-0.048907
62	1	0	-5.851929	-1.526519	-1.078676
63	1	0	-6.598243	-1.390970	0.530582
64	1	0	-6.074864	-2.962083	-0.053209
65	6	0	-3.344191	-2.409830	-0.173140
66	6	0	-1.132175	-3.703928	-1.338582
67	6	0	-3.526118	-3.500507	-1.023879
68	6	0	-2.035628	-1.986000	0.042041
69	6	0	-0.912466	-2.612874	-0.496145
70	6	0	-2.430445	-4.134433	-1.607923
71	1	0	-4.526485	-3.862564	-1.237528
72	1	0	-2.589939	-4.979684	-2.269824
73	1	0	-0.285921	-4.215856	-1.786410
74	15	0	-0.409410	1.654599	1.070240

75	15	0	0.718832	-1.890950	-0.042464
76	6	0	1.869504	-3.102127	-0.809029
77	6	0	3.623941	-4.861061	-2.091655
78	6	0	2.578328	-2.690941	-1.942390
79	6	0	2.053352	-4.400378	-0.318126
80	6	0	2.925459	-5.275643	-0.957196
81	6	0	3.451336	-3.569809	-2.582554
82	1	0	2.458544	-1.672431	-2.307704
83	1	0	1.511712	-4.720662	0.568851
84	1	0	3.063757	-6.280366	-0.569394
85	1	0	4.001252	-3.242179	-3.459642
86	1	0	4.307642	-5.544263	-2.586616
87	6	0	0.819970	-2.381882	1.737574
88	6	0	1.147704	-3.027300	4.449762
89	6	0	-0.157785	-3.114131	2.418263
90	6	0	1.965588	-1.980520	2.436333
91	6	0	2.129953	-2.301080	3.779795
92	6	0	0.005611	-3.433071	3.765632
93	1	0	-1.050657	-3.450947	1.898816
94	1	0	2.737733	-1.415461	1.921902
95	1	0	3.022898	-1.976065	4.305234
96	1	0	-0.763656	-4.003613	4.278313
97	1	0	1.271360	-3.271910	5.500666
98	6	0	-0.246987	3.481012	1.047364
99	6	0	0.039146	6.258707	0.920583
100	6	0	0.350211	4.078228	-0.065763
101	6	0	-0.694748	4.287325	2.101631
102	6	0	-0.554068	5.669626	2.037403
103	6	0	0.490908	5.463822	-0.128578
104	1	0	0.709043	3.453780	-0.880603
105	1	0	-1.147570	3.827515	2.976930
106	1	0	-0.901141	6.287365	2.859904
107	1	0	0.961010	5.918948	-0.994701
108	1	0	0.154212	7.337367	0.873757
109	6	0	-0.056702	1.251871	2.832454
110	6	0	0.656640	0.600960	5.465428
111	6	0	-0.764522	0.275598	3.538896
112	6	0	1.016292	1.897212	3.461804
113	6	0	1.368786	1.574623	4.768661
114	6	0	-0.408762	-0.045463	4.846782
115	1	0	-1.592944	-0.248369	3.076044
116	1	0	1.578989	2.657067	2.926699
117	1	0	2.201163	2.086806	5.241498
118	1	0	-0.964297	-0.812801	5.377112
119	1	0	0.932269	0.346897	6.484604

Zero-point correction=	0.994380
(Hartree/Particle)	
Thermal correction to Energy=	1.051876
Thermal correction to Enthalpy=	1.052820
Thermal correction to Gibbs Free Energy=	0.903618
Sum of electronic and zero-point Energies=	-3209.791984
Sum of electronic and thermal Energies=	-3209.734487
Sum of electronic and thermal Enthalpies=	-3209.733543
Sum of electronic and thermal Free Energies=	-3209.882746

VIIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.347434	0.706661	-2.791540
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3	6	0	-3.453790	0.581904	-1.644748
4	6	0	-3.317362	0.744017	-0.134287
5	6	0	-4.697659	1.051498	0.414206
6	7	0	-5.516604	1.298550	-0.772246
7	1	0	-5.262996	-0.635061	-1.617978
8	1	0	-4.713403	1.920789	1.086895
9	1	0	-5.082029	0.184003	0.997183
10	6	0	-6.929364	1.105161	-0.547349
11	1	0	-7.282134	1.792192	0.228630
12	1	0	-7.487983	1.311099	-1.466493
13	6	0	-2.200020	0.573106	0.581045
14	6	0	-2.295360	0.670047	2.091445
15	1	0	-1.326726	0.516006	2.582276
16	1	0	-2.988502	-0.089637	2.485743
17	1	0	-2.673708	1.649319	2.420980
18	28	0	-0.532674	0.174085	-0.409441
19	5	0	1.174788	-0.239284	-1.485905
20	8	0	1.331684	-0.301807	-2.873085
21	6	0	2.732075	-0.483838	-3.182453
22	6	0	3.288885	-1.088932	-1.857603
23	8	0	2.383553	-0.552748	-0.882304
24	1	0	-2.926044	-0.320874	-1.988116
25	6	0	-2.918367	1.788073	-2.418565
26	1	0	-1.860080	1.949603	-2.181744
27	1	0	-3.476458	2.688922	-2.139979
28	1	0	-3.007657	1.646013	-3.502518
29	6	0	3.315454	0.894054	-3.487206
30	1	0	2.750019	1.350157	-4.305894
31	1	0	4.366197	0.825313	-3.787199
32	1	0	3.240229	1.551412	-2.614343
33	6	0	2.847763	-1.390661	-4.397845
34	1	0	2.428644	-0.886666	-5.273903
35	1	0	2.301874	-2.325205	-4.245259
36	1	0	3.897090	-1.626217	-4.607699
37	6	0	4.699762	-0.658403	-1.481987
38	1	0	5.425453	-0.974568	-2.239706
39	1	0	4.969608	-1.124864	-0.528393
40	1	0	4.761931	0.424997	-1.355027
41	6	0	3.168779	-2.610914	-1.793097
42	1	0	2.149282	-2.934154	-2.033623
43	1	0	3.390070	-2.936000	-0.771395
44	1	0	3.867104	-3.101382	-2.479401
45	1	0	-7.165453	0.071775	-0.223502
46	1	0	2.682714	-5.278235	1.579348

47	6	0	2.363294	-4.241316	1.588788
48	6	0	1.558975	-1.591075	1.596925
49	6	0	3.120827	-3.283468	2.257324
50	6	0	1.195411	-3.866526	0.935930
51	6	0	0.775045	-2.533687	0.917789
52	6	0	2.722037	-1.948501	2.286368
53	1	0	4.026439	-3.587078	2.771548
54	1	0	0.613616	-4.615764	0.408288
55	6	0	3.425073	-0.861594	3.088180
56	8	0	1.159261	-0.271306	1.595344
57	6	0	2.632605	-0.641031	4.397474
58	1	0	2.635439	-1.557366	4.997071
59	1	0	1.593977	-0.368369	4.186520
60	1	0	3.091243	0.164664	4.980396
61	6	0	4.862851	-1.240444	3.442836
62	1	0	5.470024	-1.406731	2.546666
63	1	0	4.880445	-2.148343	4.051569
64	1	0	5.328994	-0.452714	4.040944
65	6	0	3.350112	0.420043	2.269528
66	6	0	2.969638	2.825446	0.891068
67	6	0	4.367336	1.369626	2.203209
68	6	0	2.155441	0.684419	1.595015
69	6	0	1.932385	1.889165	0.913678
70	6	0	4.184329	2.564788	1.514348
71	1	0	5.313922	1.182178	2.698340
72	1	0	4.984733	3.296162	1.471205
73	1	0	2.831713	3.761118	0.358546
74	15	0	-0.749402	-2.013399	0.024479
75	15	0	0.334712	2.185747	0.049355
76	6	0	0.709976	3.427845	-1.250435
77	6	0	1.232651	5.283499	-3.279353
78	6	0	0.784154	3.014305	-2.583730
79	6	0	0.879354	4.785469	-0.945223
80	6	0	1.146165	5.705831	-1.953145
81	6	0	1.048914	3.940164	-3.592519
82	1	0	0.636310	1.966424	-2.832841
83	1	0	0.791130	5.123875	0.083946
84	1	0	1.278233	6.754498	-1.705356
85	1	0	1.101332	3.607925	-4.625017
86	1	0	1.432243	6.004321	-4.066377
87	6	0	-0.597042	3.217529	1.249645
88	6	0	-2.221971	4.644069	3.021678
89	6	0	-0.198652	3.403313	2.572595
90	6	0	-1.814837	3.758328	0.815009
91	6	0	-2.620146	4.470219	1.694336
92	6	0	-1.012083	4.114277	3.456845
93	1	0	0.742787	2.988985	2.922759
94	1	0	-2.140589	3.598279	-0.209683
95	1	0	-3.563830	4.880570	1.347936
96	1	0	-0.696194	4.249977	4.486767
97	1	0	-2.855613	5.193367	3.711421
98	6	0	-0.977959	-3.281909	-1.285761
99	6	0	-1.296211	-5.170817	-3.328380
100	6	0	-0.624100	-2.966496	-2.602450
101	6	0	-1.515827	-4.545616	-1.007577
102	6	0	-1.668759	-5.485529	-2.022352
103	6	0	-0.777772	-3.911690	-3.616517

104	1	0	-0.223298	-1.983797	-2.836756
105	1	0	-1.824659	-4.791354	0.005124
106	1	0	-2.085312	-6.461920	-1.794596
107	1	0	-0.500186	-3.655085	-4.634477
108	1	0	-1.420707	-5.903995	-4.119332
109	6	0	-2.072030	-2.479724	1.211663
110	6	0	-4.188673	-2.950054	2.981127
111	6	0	-1.817188	-2.814149	2.541140
112	6	0	-3.399284	-2.388483	0.771102
113	6	0	-4.449962	-2.625496	1.647746
114	6	0	-2.874340	-3.047570	3.423170
115	1	0	-0.794554	-2.885863	2.900492
116	1	0	-3.608785	-2.114301	-0.260393
117	1	0	-5.473827	-2.546472	1.293768
118	1	0	-2.663935	-3.301934	4.457548
119	1	0	-5.009685	-3.126476	3.669286

Zero-point correction= 0.999738
(Hartree/Particle)
Thermal correction to Energy= 1.057288
Thermal correction to Enthalpy= 1.058232
Thermal correction to Gibbs Free Energy= 0.908939
Sum of electronic and zero-point Energies= -3209.859026
Sum of electronic and thermal Energies= -3209.801476
Sum of electronic and thermal Enthalpies= -3209.800532
Sum of electronic and thermal Free Energies= -3209.949825

$TS_{IIIa\text{-}VIIa}$

Imaginary frequency: -1006.4562

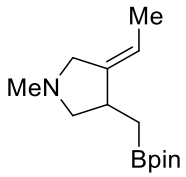
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.852651	0.413745	-3.212712
2	6	0	-4.906861	0.479769	-2.119267
3	6	0	-3.526061	0.380754	-1.430314
4	6	0	-3.530249	1.520129	-0.436159
5	6	0	-4.962667	1.989939	-0.340169
6	7	0	-5.439068	1.781994	-1.711160
7	1	0	-5.564657	-0.339064	-1.766074
8	1	0	-5.078927	3.039143	-0.050075
9	1	0	-5.547922	1.373393	0.378844
10	6	0	-6.874082	1.872075	-1.845702
11	1	0	-7.217681	2.865510	-1.539381
12	1	0	-7.160771	1.718121	-2.891377
13	6	0	-2.372296	2.010013	0.029185
14	6	0	-2.386058	3.154691	1.014049
15	1	0	-2.232508	2.793208	2.040265
16	1	0	-3.335911	3.707595	1.004887
17	1	0	-1.582896	3.878173	0.823246
18	28	0	-0.852903	1.029088	-0.835629
19	5	0	0.613239	0.012169	-2.127141
20	8	0	1.264587	0.613156	-3.174614
21	6	0	2.377445	-0.230378	-3.566255
22	6	0	1.985689	-1.614654	-2.948139
23	8	0	1.127948	-1.232914	-1.846809

24	1	0	-3.470861	-0.584716	-0.908796
25	6	0	-2.302178	0.529338	-2.325665
26	1	0	-0.807538	0.173942	-2.157528
27	1	0	-2.314680	1.493116	-2.847848
28	1	0	-2.269048	-0.266769	-3.082664
29	6	0	3.635937	0.350549	-2.938540
30	1	0	3.728297	1.402633	-3.224071
31	1	0	4.529483	-0.185974	-3.274016
32	1	0	3.581684	0.292917	-1.850395
33	6	0	2.482176	-0.213617	-5.083126
34	1	0	2.756773	0.790826	-5.417507
35	1	0	1.534994	-0.484603	-5.553940
36	1	0	3.256836	-0.910996	-5.420078
37	6	0	3.145130	-2.434200	-2.404353
38	1	0	3.831760	-2.709371	-3.212942
39	1	0	2.755862	-3.350651	-1.949216
40	1	0	3.699829	-1.885691	-1.638682
41	6	0	1.138156	-2.470553	-3.889103
42	1	0	0.273584	-1.906348	-4.257706
43	1	0	0.772693	-3.344512	-3.341269
44	1	0	1.720231	-2.817246	-4.748165
45	1	0	-7.403437	1.117821	-1.230640
46	1	0	1.668869	-5.885805	0.496428
47	6	0	1.665353	-4.810004	0.639150
48	6	0	1.665448	-2.075329	0.988706
49	6	0	2.853870	-4.143640	0.923068
50	6	0	0.471918	-4.098819	0.545796
51	6	0	0.450109	-2.713157	0.717678
52	6	0	2.873214	-2.761388	1.113907
53	1	0	3.774634	-4.712145	0.998108
54	1	0	-0.454037	-4.620379	0.320580
55	6	0	4.108389	-1.971201	1.526188
56	8	0	1.630066	-0.705374	1.133685
57	6	0	4.065877	-1.786721	3.060711
58	1	0	4.095488	-2.763050	3.556162
59	1	0	3.150797	-1.270115	3.367005
60	1	0	4.925256	-1.193855	3.391517
61	6	0	5.403960	-2.691359	1.149542
62	1	0	5.479524	-2.847492	0.068123
63	1	0	5.459908	-3.662750	1.647389
64	1	0	6.274400	-2.121132	1.484013
65	6	0	4.013543	-0.586357	0.895227
66	6	0	3.707021	2.063322	0.033881
67	6	0	5.120585	0.170187	0.510086
68	6	0	2.751630	0.010094	0.805174
69	6	0	2.568608	1.345076	0.411875
70	6	0	4.969745	1.482042	0.074643
71	1	0	6.113807	-0.262872	0.557111
72	1	0	5.837241	2.055100	-0.235489
73	1	0	3.608730	3.075258	-0.337190
74	15	0	-1.054411	-1.669638	0.492940
75	15	0	0.849995	2.034395	0.369566
76	6	0	1.065912	3.730375	-0.293605
77	6	0	1.251452	6.295494	-1.412442
78	6	0	0.272991	4.089341	-1.389724
79	6	0	1.952557	4.680445	0.236774
80	6	0	2.044873	5.952205	-0.318438

81	6	0	0.366175	5.364135	-1.945835
82	1	0	-0.435213	3.371198	-1.797672
83	1	0	2.579437	4.425425	1.086749
84	1	0	2.736353	6.674868	0.103163
85	1	0	-0.257169	5.625962	-2.794676
86	1	0	1.324798	7.288401	-1.845217
87	6	0	0.453631	2.247275	2.161402
88	6	0	-0.370220	2.414683	4.839743
89	6	0	-0.029802	1.121629	2.835278
90	6	0	0.500570	3.466410	2.843368
91	6	0	0.095528	3.545650	4.174275
92	6	0	-0.436034	1.199140	4.163657
93	1	0	-0.114525	0.180035	2.311799
94	1	0	0.809177	4.373835	2.338689
95	1	0	0.131079	4.502783	4.685712
96	1	0	-0.825088	0.308760	4.650925
97	1	0	-0.694574	2.485208	5.873532
98	6	0	-2.130990	-2.824542	-0.454777
99	6	0	-3.752732	-4.407780	-2.103201
100	6	0	-1.877989	-2.916393	-1.829939
101	6	0	-3.206997	-3.533472	0.084796
102	6	0	-4.014948	-4.318133	-0.739164
103	6	0	-2.676316	-3.707532	-2.648168
104	1	0	-1.048451	-2.354426	-2.250760
105	1	0	-3.422900	-3.469355	1.147557
106	1	0	-4.852119	-4.860201	-0.309427
107	1	0	-2.465819	-3.768662	-3.712271
108	1	0	-4.385594	-5.017763	-2.740399
109	6	0	-1.835452	-1.725584	2.160794
110	6	0	-3.158809	-1.652195	4.627511
111	6	0	-1.486297	-2.621097	3.175811
112	6	0	-2.842818	-0.779548	2.398987
113	6	0	-3.507434	-0.752047	3.621699
114	6	0	-2.143246	-2.580481	4.405696
115	1	0	-0.701166	-3.353327	3.006953
116	1	0	-3.082725	-0.046335	1.628481
117	1	0	-4.285812	-0.014713	3.793445
118	1	0	-1.863560	-3.278710	5.189139
119	1	0	-3.671043	-1.625023	5.584691

Zero-point correction= 0.996196
(Hartree/Particle)
Thermal correction to Energy= 1.053159
Thermal correction to Enthalpy= 1.054103
Thermal correction to Gibbs Free Energy= 0.906562
Sum of electronic and zero-point Energies= -3209.795207
Sum of electronic and thermal Energies= -3209.738244
Sum of electronic and thermal Enthalpies= -3209.737300
Sum of electronic and thermal Free Energies= -3209.884841

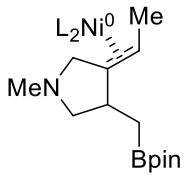
2A



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.153086	-0.527651	-0.545367
2	8	0	-1.902794	-0.716347	-1.242999
3	5	0	-0.894176	-0.501726	-0.335857
4	8	0	-1.356626	0.022007	0.848616
5	6	0	-2.734335	0.401297	0.638189
6	6	0	-3.513833	0.187382	1.925115
7	1	0	-3.155910	0.881960	2.690272
8	1	0	-3.390700	-0.830014	2.301393
9	1	0	-4.580090	0.376917	1.761672
10	6	0	-2.729726	1.880870	0.257837
11	1	0	-2.181975	2.042425	-0.676511
12	1	0	-2.230580	2.445178	1.050620
13	1	0	-3.745811	2.269013	0.139620
14	6	0	-3.615603	-1.906399	-0.077838
15	1	0	-2.896920	-2.341904	0.623622
16	1	0	-3.690578	-2.566174	-0.946434
17	1	0	-4.594023	-1.855982	0.409374
18	6	0	-4.168932	0.075146	-1.502356
19	1	0	-3.785296	0.985072	-1.967999
20	1	0	-5.099276	0.312630	-0.975182
21	1	0	-4.397750	-0.644326	-2.293617
22	6	0	0.620339	-0.813542	-0.609436
23	1	0	0.919611	-0.362629	-1.565011
24	1	0	0.750180	-1.895977	-0.742893
25	6	0	1.560318	-0.308588	0.497445
26	1	0	1.234219	-0.708709	1.463073
27	6	0	3.014668	-0.658994	0.218409
28	6	0	3.708484	0.602333	-0.257750
29	1	0	4.301384	0.464645	-1.169490
30	1	0	4.394657	0.974462	0.531349
31	7	0	2.611910	1.538190	-0.491333
32	6	0	1.619036	1.224161	0.530359
33	1	0	0.659248	1.699717	0.300199
34	1	0	1.944010	1.575775	1.529582
35	6	0	3.029872	2.921471	-0.489919
36	1	0	3.766963	3.088848	-1.281488
37	1	0	3.483837	3.222996	0.473522
38	1	0	2.168957	3.569274	-0.681663
39	6	0	3.570812	-1.856973	0.383630
40	6	0	5.006357	-2.196593	0.104834
41	1	0	5.565286	-1.328397	-0.254964
42	1	0	5.087649	-2.987948	-0.649238
43	1	0	5.505486	-2.566502	1.007971
44	1	0	2.944074	-2.667859	0.756981

Zero-point correction=	0.395059
(Hartree/Particle)	
Thermal correction to Energy=	0.414789
Thermal correction to Enthalpy=	0.415733
Thermal correction to Gibbs Free Energy=	0.347067
Sum of electronic and zero-point Energies=	-778.541735
Sum of electronic and thermal Energies=	-778.522005
Sum of electronic and thermal Enthalpies=	-778.521061
Sum of electronic and thermal Free Energies=	-778.589727

2A-Ni



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.542292	3.193679	-4.966432
2	6	0	-2.557611	2.440736	-4.184900
3	6	0	-2.611177	0.543746	-2.204735
4	6	0	-3.147496	1.202176	-4.430405
5	6	0	-1.975731	2.716923	-2.951130
6	6	0	-1.974912	1.756159	-1.934227
7	6	0	-3.190348	0.228608	-3.434463
8	1	0	-3.579056	1.001805	-5.405608
9	1	0	-1.500717	3.678445	-2.785209
10	6	0	-3.855172	-1.139077	-3.560833
11	8	0	-2.648001	-0.381004	-1.186036
12	6	0	-5.237543	-1.068835	-2.873212
13	1	0	-5.870530	-0.333107	-3.380491
14	1	0	-5.138534	-0.777929	-1.823020
15	1	0	-5.727767	-2.046984	-2.916877
16	6	0	-4.044314	-1.556755	-5.017957
17	1	0	-3.088239	-1.617885	-5.547606
18	1	0	-4.689461	-0.844494	-5.539966
19	1	0	-4.538596	-2.530801	-5.072988
20	6	0	-2.986391	-2.126747	-2.786264
21	6	0	-1.467127	-3.812978	-1.128283
22	6	0	-2.732692	-3.446210	-3.157436
23	6	0	-2.444283	-1.685890	-1.578505
24	6	0	-1.687306	-2.491405	-0.728586
25	6	0	-1.980252	-4.282860	-2.334560
26	1	0	-3.123532	-3.831526	-4.093481
27	1	0	-1.792768	-5.308265	-2.636628
28	1	0	-0.876187	-4.470933	-0.497628
29	15	0	-1.058790	1.922831	-0.338298
30	15	0	-1.042218	-1.726273	0.825978
31	6	0	0.167294	-3.017241	1.328143
32	6	0	2.197144	-4.842737	1.964090
33	6	0	1.413031	-2.956795	0.685625
34	6	0	-0.040816	-3.989816	2.307542
35	6	0	0.972809	-4.897154	2.623109

36	6	0	2.418424	-3.866029	0.991950
37	1	0	1.610484	-2.173228	-0.045747
38	1	0	-0.989762	-4.041186	2.833448
39	1	0	0.801366	-5.647220	3.389392
40	1	0	3.375721	-3.786414	0.484855
41	1	0	2.981951	-5.549969	2.214868
42	6	0	-2.498170	-1.955879	1.926316
43	6	0	-4.712168	-2.179914	3.622857
44	6	0	-3.262786	-3.130097	1.943442
45	6	0	-2.871138	-0.888483	2.747717
46	6	0	-3.972834	-1.001681	3.594936
47	6	0	-4.358918	-3.244044	2.792095
48	1	0	-3.000909	-3.955458	1.285066
49	1	0	-2.304424	0.039720	2.715963
50	1	0	-4.252797	-0.160871	4.222240
51	1	0	-4.942888	-4.159314	2.801758
52	1	0	-5.570416	-2.268700	4.282238
53	6	0	-0.296094	3.575656	-0.589009
54	6	0	1.018007	6.002942	-1.064767
55	6	0	-0.859916	4.780046	-0.159725
56	6	0	0.930126	3.601728	-1.262554
57	6	0	1.580644	4.806955	-1.508309
58	6	0	-0.200010	5.986651	-0.389490
59	1	0	-1.813964	4.777868	0.359699
60	1	0	1.381815	2.665585	-1.586806
61	1	0	2.532857	4.811343	-2.030318
62	1	0	-0.641957	6.915853	-0.042759
63	1	0	1.528902	6.944212	-1.242518
64	6	0	-2.387720	2.252169	0.891871
65	6	0	-4.261525	2.538066	2.958193
66	6	0	-3.736505	1.969728	0.667426
67	6	0	-1.987710	2.685449	2.164999
68	6	0	-2.917626	2.833806	3.189083
69	6	0	-4.665832	2.107211	1.698101
70	1	0	-4.070669	1.636656	-0.310472
71	1	0	-0.938344	2.905258	2.351501
72	1	0	-2.591190	3.173542	4.167528
73	1	0	-5.710039	1.875610	1.511419
74	1	0	-4.989184	2.645427	3.757016
75	6	0	6.523879	-0.804352	-1.221565
76	8	0	5.961782	-0.069459	-0.113250
77	5	0	4.772685	-0.673121	0.220174
78	8	0	4.404418	-1.635710	-0.699718
79	6	0	5.259443	-1.469129	-1.849746
80	6	0	5.500517	-2.823656	-2.494997
81	1	0	4.560327	-3.209285	-2.899487
82	1	0	5.884243	-3.545418	-1.770845
83	1	0	6.217573	-2.734729	-3.318243
84	6	0	4.523642	-0.538197	-2.812384
85	1	0	4.363225	0.444071	-2.354107
86	1	0	3.546364	-0.971314	-3.043538
87	1	0	5.077657	-0.403178	-3.746173
88	6	0	7.497056	-1.823712	-0.632657
89	1	0	6.971876	-2.538648	0.008658
90	1	0	8.235049	-1.294914	-0.023507
91	1	0	8.022844	-2.375035	-1.417967
92	6	0	7.258932	0.161722	-2.136705

93	1	0	6.620058	0.997360	-2.429793
94	1	0	7.603238	-0.353605	-3.039929
95	1	0	8.133581	0.564955	-1.618450
96	6	0	3.836410	-0.271194	1.404197
97	1	0	4.370813	0.126446	2.273956
98	1	0	3.289169	-1.163569	1.723660
99	6	0	2.846361	0.809263	0.905302
100	1	0	2.501895	0.530996	-0.103153
101	6	0	1.643719	1.062224	1.844393
102	6	0	1.772549	2.503581	2.317266
103	1	0	1.477480	2.642484	3.365162
104	1	0	1.179670	3.210810	1.701369
105	7	0	3.199174	2.788163	2.149147
106	6	0	3.530358	2.187973	0.860745
107	1	0	4.617363	2.117999	0.733059
108	1	0	3.126492	2.798881	0.031883
109	6	0	3.497625	4.202495	2.199277
110	1	0	3.223383	4.606227	3.179362
111	1	0	2.948617	4.772494	1.423902
112	1	0	4.570415	4.362857	2.050834
113	6	0	1.076794	0.024215	2.599330
114	6	0	0.326021	0.249680	3.894159
115	1	0	-0.312858	1.139044	3.860184
116	1	0	1.017505	0.372535	4.740589
117	1	0	-0.319830	-0.605388	4.124073
118	28	0	-0.002864	0.313874	0.926053
119	1	0	1.525068	-0.966003	2.529959

Zero-point correction= 1.002152
(Hartree/Particle)
Thermal correction to Energy= 1.059407
Thermal correction to Enthalpy= 1.060351
Thermal correction to Gibbs Free Energy= 0.909839
Sum of electronic and zero-point Energies= -3209.896540
Sum of electronic and thermal Energies= -3209.839286
Sum of electronic and thermal Enthalpies= -3209.838342
Sum of electronic and thermal Free Energies= -3209.988854

$TS_{IVa\text{-}2A}$

Imaginary frequencies = -604.92 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.249466	0.192056	0.283197
2	1	0	3.879452	0.733691	2.915441
3	6	0	3.372398	0.621793	1.945693
4	1	0	2.517223	-0.041507	2.129067
5	6	0	2.876934	1.992471	1.457145
6	6	0	3.941190	3.093763	1.549773
7	7	0	3.562523	4.041278	0.504394
8	6	0	3.222978	3.201573	-0.645763
9	6	0	2.485466	2.035050	-0.017674
10	1	0	2.012426	2.296039	2.068170
11	1	0	4.942661	2.665440	1.353362
12	1	0	3.967486	3.588892	2.527443

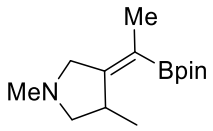
13	1	0	4.139781	2.858655	-1.171011
14	1	0	2.616513	3.770371	-1.363052
15	1	0	4.256227	5.692060	-0.572916
16	6	0	1.560442	1.272237	-0.617059
17	6	0	4.594666	5.012029	0.215775
18	1	0	4.809623	5.604728	1.110903
19	1	0	5.536364	4.536462	-0.118613
20	1	0	1.579305	-0.342252	-0.195657
21	5	0	4.310735	-0.092633	0.905093
22	8	0	5.163396	0.546603	0.034357
23	6	0	5.542750	-0.417940	-0.968585
24	6	0	5.396140	-1.768992	-0.196933
25	8	0	4.357346	-1.461540	0.754593
26	6	0	6.949613	-0.105691	-1.450716
27	1	0	6.952588	0.860720	-1.963313
28	1	0	7.292045	-0.869628	-2.157165
29	1	0	7.654516	-0.053993	-0.618342
30	6	0	4.540483	-0.282088	-2.114406
31	1	0	4.554861	0.752866	-2.469564
32	1	0	3.523399	-0.504741	-1.774084
33	1	0	4.793650	-0.943317	-2.949191
34	6	0	6.643177	-2.133095	0.605265
35	1	0	6.973242	-1.286148	1.214828
36	1	0	7.466037	-2.438521	-0.048054
37	1	0	6.403171	-2.964919	1.273956
38	6	0	4.945190	-2.943980	-1.050299
39	1	0	3.961671	-2.758313	-1.488170
40	1	0	4.879633	-3.845256	-0.433182
41	1	0	5.664004	-3.132438	-1.855126
42	1	0	-2.696522	3.638592	-4.134471
43	6	0	-2.618547	2.745209	-3.523458
44	6	0	-2.412610	0.486537	-1.984451
45	6	0	-2.792382	1.491729	-4.107560
46	6	0	-2.332897	2.862599	-2.165760
47	6	0	-2.211819	1.721948	-1.366514
48	6	0	-2.702492	0.331501	-3.339789
49	1	0	-3.002708	1.424653	-5.169893
50	1	0	-2.173742	3.843955	-1.730563
51	6	0	-2.952328	-1.086459	-3.849319
52	8	0	-2.301105	-0.627058	-1.184386
53	6	0	-4.389304	-1.491202	-3.447511
54	1	0	-5.114878	-0.818344	-3.916400
55	1	0	-4.520120	-1.440407	-2.361447
56	1	0	-4.594850	-2.516480	-3.772596
57	6	0	-2.808973	-1.187610	-5.366832
58	1	0	-1.804366	-0.903711	-5.695819
59	1	0	-3.537486	-0.540980	-5.863864
60	1	0	-3.012167	-2.208821	-5.701298
61	6	0	-1.984318	-2.010775	-3.116105
62	6	0	-0.366523	-3.672655	-1.513198
63	6	0	-1.373000	-3.144617	-3.653306
64	6	0	-1.740545	-1.738859	-1.772510
65	6	0	-0.943771	-2.534340	-0.949520
66	6	0	-0.576728	-3.968646	-2.859096
67	1	0	-1.520442	-3.395609	-4.698604
68	1	0	-0.116768	-4.849928	-3.294224
69	1	0	0.260758	-4.315304	-0.902428

70	15	0	-1.571356	1.727053	0.364469
71	15	0	-0.644024	-1.902045	0.749908
72	6	0	0.396101	-3.228979	1.476021
73	6	0	2.094916	-5.194381	2.509797
74	6	0	1.781806	-3.052520	1.445262
75	6	0	-0.136054	-4.400433	2.026962
76	6	0	0.712400	-5.378080	2.540245
77	6	0	2.628504	-4.031505	1.960142
78	1	0	2.203759	-2.150622	1.013668
79	1	0	-1.212381	-4.547154	2.058617
80	1	0	0.293475	-6.283949	2.967958
81	1	0	3.701174	-3.862619	1.938237
82	1	0	2.751860	-5.956440	2.918564
83	6	0	-2.261417	-2.200097	1.568465
84	6	0	-4.630816	-2.657149	2.984509
85	6	0	-3.291766	-2.951077	0.997382
86	6	0	-2.437376	-1.663732	2.848677
87	6	0	-3.609618	-1.901071	3.557514
88	6	0	-4.473670	-3.174148	1.701819
89	1	0	-3.170204	-3.373559	0.003470
90	1	0	-1.652388	-1.051795	3.288913
91	1	0	-3.735255	-1.476718	4.548785
92	1	0	-5.268422	-3.759049	1.248238
93	1	0	-5.550860	-2.833959	3.533738
94	6	0	-1.373157	3.529469	0.673521
95	6	0	-0.998015	6.271553	1.086419
96	6	0	-0.088724	4.077586	0.663317
97	6	0	-2.474439	4.369546	0.889249
98	6	0	-2.286143	5.732521	1.091767
99	6	0	0.099126	5.443668	0.872719
100	1	0	0.768765	3.436258	0.487643
101	1	0	-3.478647	3.953451	0.902974
102	1	0	-3.144571	6.376210	1.259186
103	1	0	1.111140	5.837791	0.872110
104	1	0	-0.855958	7.335439	1.252024
105	6	0	-3.050630	1.382479	1.405918
106	6	0	-5.222234	0.933861	3.116797
107	6	0	-4.213307	0.777045	0.926289
108	6	0	-2.977472	1.737956	2.759280
109	6	0	-4.059052	1.525369	3.606632
110	6	0	-5.291369	0.550999	1.781152
111	1	0	-4.290382	0.490290	-0.118181
112	1	0	-2.076169	2.208578	3.146651
113	1	0	-3.993642	1.822113	4.649278
114	1	0	-6.189776	0.078076	1.396037
115	1	0	-6.066869	0.762512	3.777663
116	1	0	0.776513	0.586766	-2.528199
117	1	0	2.165224	1.679353	-2.680656
118	1	0	0.570846	2.310308	-2.228469
119	6	0	1.263448	1.466252	-2.090522

Zero-point correction= 0.995533
(Hartree/Particle)
Thermal correction to Energy= 1.052758
Thermal correction to Enthalpy= 1.053702
Thermal correction to Gibbs Free Energy= 0.904354
Sum of electronic and zero-point Energies= -3209.866612

Sum of electronic and thermal Energies= -3209.809387
Sum of electronic and thermal Enthalpies= -3209.808443
Sum of electronic and thermal Free Energies= -3209.957790

11A



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.805795	0.529689	-0.181568
2	6	0	1.946300	-0.957505	-0.454702
3	6	0	3.382829	-1.039902	-1.017151
4	7	0	4.157229	0.067340	-0.441282
5	6	0	3.190916	1.153893	-0.270065
6	1	0	1.214339	-1.278923	-1.201483
7	1	0	3.872846	-1.996426	-0.810004
8	1	0	3.353836	-0.908950	-2.106683
9	1	0	3.220583	1.832844	-1.137225
10	1	0	3.436337	1.761548	0.609461
11	6	0	4.859180	-0.256787	0.792884
12	1	0	4.204225	-0.424094	1.664066
13	1	0	5.540381	0.562588	1.044064
14	1	0	5.462441	-1.156055	0.639850
15	6	0	0.685609	1.233645	0.059392
16	6	0	1.736208	-1.803507	0.808184
17	1	0	0.708820	-1.694999	1.164715
18	1	0	2.412137	-1.502471	1.613307
19	6	0	0.785743	2.723627	0.326175
20	1	0	-0.202839	3.177024	0.424351
21	1	0	1.315797	3.241769	-0.482991
22	1	0	1.339411	2.929851	1.250788
23	5	0	-0.726585	0.592099	0.031615
24	8	0	-1.858935	1.300199	0.366596
25	8	0	-1.016864	-0.702443	-0.342503
26	6	0	-2.996463	0.499625	-0.014443
27	6	0	-2.399393	-0.944184	-0.007106
28	6	0	-4.122446	0.730140	0.980701
29	1	0	-4.966550	0.066278	0.764850
30	1	0	-4.472377	1.763566	0.904762
31	1	0	-3.789910	0.555513	2.005839
32	6	0	-3.417672	0.957064	-1.409597
33	1	0	-4.318566	0.435455	-1.746143
34	1	0	-2.617870	0.781189	-2.135705
35	1	0	-3.625692	2.030040	-1.380839
36	6	0	-2.418623	-1.582456	1.380424
37	1	0	-3.436146	-1.843193	1.686538
38	1	0	-1.817097	-2.495672	1.358904
39	6	0	-3.000260	-1.889715	-1.034659
40	1	0	-4.073431	-2.017526	-0.856711
41	1	0	-2.521388	-2.869755	-0.954500
42	1	0	-2.853326	-1.518137	-2.050725

43	1	0	-1.990516	-0.904973	2.126518
44	1	0	1.916943	-2.862169	0.592333

Zero-point correction= 0.395277
(Hartree/Particle)
Thermal correction to Energy= 0.415304
Thermal correction to Enthalpy= 0.416248
Thermal correction to Gibbs Free Energy= 0.347156
Sum of electronic and zero-point Energies= -778.542452
Sum of electronic and thermal Energies= -778.522425
Sum of electronic and thermal Enthalpies= -778.521481
Sum of electronic and thermal Free Energies= -778.590573

$TS_{Va\text{-}11A}$

Imaginary frequencies = -778.2777 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.589448	2.926392	-0.900658
2	6	0	-5.863199	2.140380	-0.721095
3	6	0	-4.026469	0.152867	-0.271029
4	6	0	-6.226515	0.808560	-0.909203
5	6	0	-4.574599	2.472450	-0.313045
6	6	0	-3.619513	1.475579	-0.085894
7	6	0	-5.309443	-0.215276	-0.679127
8	1	0	-7.233581	0.572673	-1.237059
9	1	0	-4.302926	3.515748	-0.191184
10	6	0	-5.603480	-1.708424	-0.795064
11	8	0	-3.087864	-0.829138	-0.041666
12	6	0	-5.818995	-2.271199	0.628430
13	1	0	-6.687189	-1.791726	1.092546
14	1	0	-4.942719	-2.090375	1.258670
15	1	0	-5.994782	-3.350951	0.581218
16	6	0	-6.847580	-1.989267	-1.635840
17	1	0	-6.740620	-1.604934	-2.655161
18	1	0	-7.728945	-1.530634	-1.178814
19	1	0	-7.039165	-3.064881	-1.684513
20	6	0	-4.353468	-2.359249	-1.379290
21	6	0	-1.916969	-3.489316	-2.217501
22	6	0	-4.335729	-3.418484	-2.286114
23	6	0	-3.123327	-1.883630	-0.927986
24	6	0	-1.896265	-2.413670	-1.326544
25	6	0	-3.128951	-3.981225	-2.697482
26	1	0	-5.267846	-3.815570	-2.674433
27	1	0	-3.133519	-4.811394	-3.396344
28	1	0	-0.981962	-3.933005	-2.546096
29	15	0	-1.836520	1.789787	0.279983
30	15	0	-0.389359	-1.602873	-0.649548
31	6	0	0.943150	-2.582571	-1.448482
32	6	0	3.017971	-3.915673	-2.778009
33	6	0	1.248831	-2.277201	-2.782224
34	6	0	1.694077	-3.557650	-0.788623
35	6	0	2.728948	-4.217803	-1.450829
36	6	0	2.271974	-2.945612	-3.446376
37	1	0	0.680695	-1.506700	-3.300785

38	1	0	1.478177	-3.801229	0.247702
39	1	0	3.308945	-4.970100	-0.924581
40	1	0	2.496189	-2.700317	-4.479861
41	1	0	3.825683	-4.429186	-3.290076
42	6	0	-0.402284	-2.238494	1.073679
43	6	0	-0.317992	-3.125023	3.724740
44	6	0	-0.936539	-3.484963	1.418721
45	6	0	0.163670	-1.438833	2.069319
46	6	0	0.211249	-1.881711	3.390221
47	6	0	-0.893619	-3.925464	2.738192
48	1	0	-1.384663	-4.112234	0.651701
49	1	0	0.554781	-0.457651	1.806882
50	1	0	0.647417	-1.244725	4.154132
51	1	0	-1.310385	-4.893953	2.998001
52	1	0	-0.288675	-3.470140	4.753863
53	6	0	-1.781928	3.625819	0.221686
54	6	0	-1.669453	6.411676	0.007211
55	6	0	-2.307142	4.433916	1.235945
56	6	0	-1.194678	4.225901	-0.895174
57	6	0	-1.144394	5.613742	-1.006382
58	6	0	-2.248731	5.821002	1.129640
59	1	0	-2.758393	3.974236	2.112266
60	1	0	-0.758201	3.594600	-1.665893
61	1	0	-0.684065	6.070377	-1.877269
62	1	0	-2.652413	6.441809	1.923708
63	1	0	-1.621320	7.493430	-0.072680
64	6	0	-1.710830	1.471365	2.088481
65	6	0	-1.304695	0.936580	4.807926
66	6	0	-2.673701	0.778180	2.822916
67	6	0	-0.533083	1.886915	2.727893
68	6	0	-0.335740	1.628169	4.079718
69	6	0	-2.468424	0.509933	4.176506
70	1	0	-3.592425	0.447818	2.346100
71	1	0	0.231372	2.411796	2.157860
72	1	0	0.576514	1.963435	4.564965
73	1	0	-3.224904	-0.031965	4.735931
74	1	0	-1.149029	0.729858	5.862575
75	6	0	4.237218	1.357093	-1.958469
76	6	0	2.933129	1.887453	-1.365832
77	6	0	2.413571	2.824174	-2.470173
78	7	0	3.587142	3.169120	-3.260642
79	6	0	4.347778	1.928951	-3.355002
80	1	0	3.148438	2.456652	-0.454940
81	1	0	1.666673	2.278840	-3.086535
82	1	0	1.925309	3.724084	-2.078949
83	1	0	5.376242	2.128013	-3.673512
84	1	0	3.894364	1.230853	-4.093400
85	6	0	3.265811	3.743471	-4.546455
86	1	0	2.660222	3.058924	-5.172178
87	1	0	4.185100	3.982037	-5.090720
88	1	0	2.699771	4.669904	-4.407064
89	6	0	5.105336	0.522757	-1.365990
90	6	0	1.927155	0.768380	-1.054562
91	1	0	2.321614	0.140580	-0.245369
92	1	0	1.848545	0.141098	-1.955429
93	28	0	-0.030541	0.724181	-0.626508
94	1	0	0.859489	1.899211	-0.562399

95	6	0	6.303604	-0.053176	-2.090157
96	1	0	6.317435	-1.143366	-1.982208
97	1	0	7.245890	0.312921	-1.663820
98	1	0	6.304299	0.178536	-3.158563
99	5	0	4.932490	0.082767	0.115051
100	8	0	5.489827	-1.076928	0.608974
101	8	0	4.285715	0.803165	1.095322
102	6	0	4.956679	-1.271590	1.935524
103	6	0	4.595951	0.187248	2.359799
104	6	0	3.724983	-2.164727	1.795014
105	1	0	3.275717	-2.394281	2.766945
106	1	0	4.021550	-3.100773	1.312341
107	1	0	2.962672	-1.690407	1.166095
108	6	0	6.007913	-1.948248	2.800043
109	1	0	5.654854	-2.037769	3.833157
110	1	0	6.946669	-1.390722	2.795461
111	1	0	6.203954	-2.953722	2.416811
112	6	0	3.386862	0.309864	3.273418
113	1	0	3.552894	-0.231087	4.211887
114	1	0	3.212588	1.364352	3.508002
115	6	0	5.786250	0.943992	2.946362
116	1	0	6.045510	0.573885	3.943020
117	1	0	5.527007	2.003421	3.022819
118	1	0	6.663145	0.851624	2.297844
119	1	0	2.490642	-0.086163	2.791304

Zero-point correction=	0.994591
(Hartree/Particle)	
Thermal correction to Energy=	1.052448
Thermal correction to Enthalpy=	1.053392
Thermal correction to Gibbs Free Energy=	0.900231
Sum of electronic and zero-point Energies=	-3209.845850
Sum of electronic and thermal Energies=	-3209.787992
Sum of electronic and thermal Enthalpies=	-3209.787048
Sum of electronic and thermal Free Energies=	-3209.940209

$TS_{VIa\text{-}2A}$

Imaginary frequency: -104.5637

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.106186	3.672808	-2.727340
2	6	0	3.233124	3.816745	-1.648957
3	6	0	2.078156	3.209079	-0.822780
4	6	0	2.800785	2.740156	0.439733
5	6	0	4.272142	3.045356	0.269783
6	7	0	4.434421	3.132887	-1.177675
7	1	0	3.309909	4.906111	-1.455352
8	1	0	4.933421	2.274228	0.685277
9	1	0	4.530646	4.007557	0.761449
10	6	0	5.658895	3.788091	-1.578867
11	1	0	6.523478	3.241662	-1.186236
12	1	0	5.731097	3.805724	-2.670723
13	6	0	2.236473	2.152474	1.496323
14	28	0	0.086651	0.631779	-0.934358

15	5	0	-0.644431	2.352224	-0.538925
16	8	0	-0.917630	2.548912	0.819780
17	6	0	-1.406715	3.881111	1.042176
18	6	0	-1.840468	4.329791	-0.399386
19	8	0	-1.098824	3.453467	-1.261828
20	1	0	1.380457	4.018871	-0.580642
21	6	0	1.286736	2.124396	-1.564121
22	1	0	1.158656	1.999185	1.482048
23	1	0	2.004559	1.384341	-1.950445
24	1	0	0.836483	2.594802	-2.448139
25	6	0	-0.273395	4.708416	1.653380
26	1	0	0.024972	4.243588	2.598123
27	1	0	-0.597514	5.733608	1.859682
28	1	0	0.609254	4.741375	1.012395
29	6	0	-2.548306	3.827958	2.051566
30	1	0	-2.175637	3.417887	2.995115
31	1	0	-3.365428	3.192301	1.710102
32	1	0	-2.939321	4.834305	2.240765
33	6	0	-1.474821	5.767593	-0.744421
34	1	0	-1.983357	6.469527	-0.074281
35	1	0	-1.784763	5.986499	-1.770451
36	1	0	-0.396747	5.931071	-0.671194
37	6	0	-3.325177	4.096525	-0.679855
38	1	0	-3.608960	3.059939	-0.469816
39	1	0	-3.517166	4.280616	-1.740846
40	1	0	-3.956905	4.765464	-0.086725
41	1	0	5.716630	4.830165	-1.209995
42	1	0	4.008474	-1.955822	3.861656
43	6	0	3.056759	-1.867548	3.347739
44	6	0	0.652368	-1.655469	2.052081
45	6	0	1.874916	-1.826626	4.085379
46	6	0	3.031249	-1.772995	1.958338
47	6	0	1.815245	-1.651532	1.279733
48	6	0	0.639832	-1.723910	3.444821
49	1	0	1.921573	-1.882220	5.168074
50	1	0	3.962197	-1.773876	1.400832
51	6	0	-0.719800	-1.769072	4.139050
52	8	0	-0.534675	-1.606272	1.363068
53	6	0	-1.240123	-3.222965	4.060960
54	1	0	-0.557110	-3.895842	4.590193
55	1	0	-1.314780	-3.553471	3.019196
56	1	0	-2.232647	-3.293659	4.518362
57	6	0	-0.631487	-1.342751	5.603781
58	1	0	-0.259463	-0.318045	5.701053
59	1	0	0.031970	-2.011233	6.159368
60	1	0	-1.613613	-1.407443	6.080520
61	6	0	-1.681752	-0.891666	3.341567
62	6	0	-3.479722	0.468368	1.649310
63	6	0	-2.733518	-0.143097	3.872336
64	6	0	-1.559348	-0.906419	1.955422
65	6	0	-2.432567	-0.256154	1.083982
66	6	0	-3.621514	0.528843	3.034877
67	1	0	-2.870487	-0.085380	4.947220
68	1	0	-4.431503	1.108352	3.466731
69	1	0	-4.175072	1.003768	1.009599
70	15	0	1.655456	-1.336004	-0.534230
71	15	0	-1.969436	-0.358812	-0.687281

72	6	0	-3.361341	0.419888	-1.597069
73	6	0	-5.408338	1.546016	-3.132764
74	6	0	-3.060382	1.318853	-2.622747
75	6	0	-4.697527	0.066600	-1.364848
76	6	0	-5.716635	0.639852	-2.116417
77	6	0	-4.082082	1.873941	-3.393319
78	1	0	-2.025723	1.598553	-2.802084
79	1	0	-4.934995	-0.668244	-0.598482
80	1	0	-6.750345	0.371363	-1.921076
81	1	0	-3.837803	2.571535	-4.188773
82	1	0	-6.204644	1.987328	-3.724567
83	6	0	-2.356074	-2.123388	-1.074614
84	6	0	-3.046299	-4.711669	-1.887601
85	6	0	-2.976465	-3.001730	-0.183868
86	6	0	-2.067709	-2.561198	-2.371362
87	6	0	-2.419500	-3.842569	-2.779076
88	6	0	-3.315739	-4.292352	-0.589069
89	1	0	-3.209947	-2.680850	0.827895
90	1	0	-1.567439	-1.890824	-3.068161
91	1	0	-2.187989	-4.169144	-3.788316
92	1	0	-3.798556	-4.966317	0.112648
93	1	0	-3.314656	-5.715425	-2.203552
94	6	0	3.434735	-1.356563	-1.012666
95	6	0	6.171259	-1.255396	-1.608770
96	6	0	4.107245	-0.133942	-1.063361
97	6	0	4.151970	-2.536471	-1.254614
98	6	0	5.511298	-2.483326	-1.548803
99	6	0	5.466417	-0.080776	-1.366334
100	1	0	3.578042	0.790426	-0.867922
101	1	0	3.648923	-3.498159	-1.208582
102	1	0	6.056699	-3.404015	-1.733454
103	1	0	5.951521	0.889384	-1.421900
104	1	0	7.230077	-1.220205	-1.847596
105	6	0	1.123898	-2.958179	-1.224297
106	6	0	0.442737	-5.391535	-2.431415
107	6	0	0.581159	-3.994597	-0.463907
108	6	0	1.289350	-3.141278	-2.603821
109	6	0	0.963547	-4.353222	-3.201746
110	6	0	0.238554	-5.203582	-1.068095
111	1	0	0.434026	-3.869781	0.604899
112	1	0	1.705650	-2.338079	-3.209039
113	1	0	1.116340	-4.487172	-4.268618
114	1	0	-0.186192	-6.001451	-0.466202
115	1	0	0.183177	-6.338204	-2.896145
116	6	0	2.953518	1.725270	2.745108
117	1	0	2.532409	0.793382	3.134613
118	1	0	2.847725	2.480974	3.534795
119	1	0	4.024555	1.570344	2.578072

Zero-point correction= 0.999049
(Hartree/Particle)
Thermal correction to Energy= 1.056080
Thermal correction to Enthalpy= 1.057024
Thermal correction to Gibbs Free Energy= 0.908862
Sum of electronic and zero-point Energies= -3209.851530
Sum of electronic and thermal Energies= -3209.794500
Sum of electronic and thermal Enthalpies= -3209.793555

Sum of electronic and thermal Free Energies= -3209.941718

$TS_{VIIa\text{-}11A}$

Imaginary frequency: -56.6018

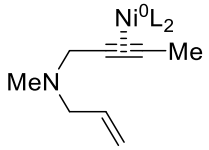
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.940229	-1.584309	-0.617052
2	6	0	-4.982142	-1.581914	-0.080071
3	6	0	-4.285889	-0.221399	-0.065875
4	6	0	-3.303572	-0.427681	1.063800
5	6	0	-4.080649	-1.241894	2.097008
6	7	0	-5.204136	-1.835555	1.344854
7	1	0	-4.324043	-2.339395	-0.549512
8	1	0	-4.469401	-0.623774	2.921081
9	1	0	-3.450866	-2.017640	2.553090
10	6	0	-5.485431	-3.214690	1.658750
11	1	0	-5.667316	-3.327724	2.732584
12	1	0	-6.388263	-3.536967	1.128158
13	6	0	-2.020229	-0.046181	1.151471
14	6	0	-1.301998	-0.255822	2.483208
15	1	0	-0.213802	-0.384646	2.375912
16	1	0	-1.667007	-1.142800	3.016986
17	1	0	-1.444836	0.616811	3.132436
18	28	0	-0.427607	0.363586	0.134690
19	5	0	-1.626706	1.836415	-0.159619
20	8	0	-2.278320	2.852808	0.529840
21	6	0	-2.593511	3.919291	-0.389447
22	6	0	-2.561166	3.211443	-1.789065
23	8	0	-1.737267	2.055783	-1.538267
24	1	0	-3.787191	0.012982	-1.010877
25	6	0	-5.289269	0.877034	0.320547
26	1	0	-4.758356	1.796411	0.581547
27	1	0	-5.871772	0.559614	1.190186
28	1	0	-5.993801	1.083731	-0.494213
29	6	0	-1.504898	4.979882	-0.231964
30	1	0	-1.467696	5.292111	0.816670
31	1	0	-1.706368	5.860770	-0.850200
32	1	0	-0.526022	4.578576	-0.503361
33	6	0	-3.940643	4.525249	-0.020110
34	1	0	-3.887628	4.938329	0.991529
35	1	0	-4.746731	3.790523	-0.049943
36	1	0	-4.189712	5.339841	-0.709404
37	6	0	-1.929765	4.043982	-2.897448
38	1	0	-2.523488	4.946375	-3.083099
39	1	0	-1.906251	3.456966	-3.821029
40	1	0	-0.910649	4.339833	-2.650976
41	6	0	-3.920850	2.716301	-2.273599
42	1	0	-4.415546	2.109880	-1.517668
43	1	0	-3.767782	2.097042	-3.163583
44	1	0	-4.577632	3.550642	-2.541035
45	1	0	-4.667113	-3.905340	1.372765
46	1	0	2.426175	-5.116629	-3.423630
47	6	0	2.465940	-4.327297	-2.679928
48	6	0	2.562653	-2.300872	-0.830547
49	6	0	3.699881	-3.869300	-2.220939

50	6	0	1.284020	-3.788559	-2.182669
51	6	0	1.309843	-2.760421	-1.234985
52	6	0	3.767715	-2.849942	-1.274986
53	1	0	4.611347	-4.313714	-2.606591
54	1	0	0.332714	-4.158685	-2.548792
55	6	0	5.046984	-2.321272	-0.634969
56	8	0	2.595738	-1.252624	0.068031
57	6	0	5.167724	-2.927644	0.781751
58	1	0	5.235691	-4.018555	0.718059
59	1	0	4.301039	-2.667968	1.397092
60	1	0	6.067468	-2.545700	1.275320
61	6	0	6.291410	-2.693247	-1.439762
62	1	0	6.255058	-2.280695	-2.453085
63	1	0	6.389614	-3.780404	-1.506885
64	1	0	7.193092	-2.324247	-0.943210
65	6	0	4.874702	-0.812686	-0.501774
66	6	0	4.361119	1.920226	-0.170355
67	6	0	5.888427	0.123255	-0.680248
68	6	0	3.605827	-0.341867	-0.145276
69	6	0	3.304913	1.013257	-0.009456
70	6	0	5.637989	1.482015	-0.496617
71	1	0	6.883913	-0.202587	-0.962927
72	1	0	6.438567	2.202767	-0.626280
73	1	0	4.174524	2.983786	-0.063369
74	15	0	-0.175963	-1.983959	-0.454034
75	15	0	1.562212	1.569173	0.302959
76	6	0	1.683417	3.242139	-0.447123
77	6	0	1.967016	5.699604	-1.756440
78	6	0	1.475383	3.336401	-1.826718
79	6	0	2.029132	4.391147	0.272388
80	6	0	2.161480	5.615174	-0.379355
81	6	0	1.632666	4.556596	-2.480191
82	1	0	1.177164	2.453646	-2.388062
83	1	0	2.193796	4.331777	1.344390
84	1	0	2.421514	6.502400	0.189646
85	1	0	1.474441	4.617537	-3.552944
86	1	0	2.075279	6.653174	-2.263835
87	6	0	1.596805	1.938903	2.105142
88	6	0	1.498179	2.487851	4.846903
89	6	0	2.634789	1.528859	2.944171
90	6	0	0.500911	2.623258	2.650952
91	6	0	0.461235	2.905171	4.012310
92	6	0	2.580499	1.796755	4.312071
93	1	0	3.491098	1.000912	2.534454
94	1	0	-0.326655	2.923174	2.009599
95	1	0	-0.389405	3.439374	4.424871
96	1	0	3.390383	1.468000	4.956133
97	1	0	1.459257	2.699495	5.911044
98	6	0	-1.522533	-2.451369	-1.607102
99	6	0	-3.576116	-2.998804	-3.429834
100	6	0	-2.087485	-1.422327	-2.366824
101	6	0	-2.002143	-3.758855	-1.765837
102	6	0	-3.022252	-4.030958	-2.672324
103	6	0	-3.107981	-1.697143	-3.276688
104	1	0	-1.748749	-0.396262	-2.225352
105	1	0	-1.584488	-4.565174	-1.167855
106	1	0	-3.389401	-5.046546	-2.783776

107	1	0	-3.546084	-0.887633	-3.853192
108	1	0	-4.376576	-3.210297	-4.132336
109	6	0	-0.405919	-3.118757	0.979097
110	6	0	-0.753896	-4.639004	3.311951
111	6	0	0.693577	-3.474860	1.769403
112	6	0	-1.681791	-3.526031	1.378713
113	6	0	-1.853260	-4.284557	2.535039
114	6	0	0.520813	-4.230181	2.925100
115	1	0	1.694127	-3.159143	1.486932
116	1	0	-2.548599	-3.239351	0.789880
117	1	0	-2.852841	-4.592042	2.830119
118	1	0	1.385300	-4.499515	3.524169
119	1	0	-0.888722	-5.227888	4.213986

Zero-point correction= 1.000428
(Hartree/Particle)
Thermal correction to Energy= 1.057127
Thermal correction to Enthalpy= 1.058072
Thermal correction to Gibbs Free Energy= 0.912417
Sum of electronic and zero-point Energies= -3209.845655
Sum of electronic and thermal Energies= -3209.788957
Sum of electronic and thermal Enthalpies= -3209.788012
Sum of electronic and thermal Free Energies= -3209.933667

Xa



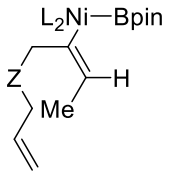
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.129940	3.219377	-2.162945
2	6	0	-4.536951	2.416874	-1.736294
3	6	0	-3.042896	0.389487	-0.658436
4	6	0	-5.047616	1.120053	-1.711308
5	6	0	-3.269405	2.691146	-1.230224
6	6	0	-2.486553	1.667377	-0.687721
7	6	0	-4.305336	0.076601	-1.161207
8	1	0	-6.032424	0.928283	-2.124834
9	1	0	-2.878083	3.702293	-1.276650
10	6	0	-4.771626	-1.370147	-1.022698
11	8	0	-2.272292	-0.605475	-0.101071
12	6	0	-5.236869	-1.591095	0.434783
13	1	0	-6.083631	-0.935120	0.662041
14	1	0	-4.429427	-1.374650	1.141593
15	1	0	-5.548678	-2.631510	0.574902
16	6	0	-5.923489	-1.697731	-1.971111
17	1	0	-5.636899	-1.552500	-3.017551
18	1	0	-6.789117	-1.065570	-1.753704
19	1	0	-6.245833	-2.734095	-1.836295
20	6	0	-3.552490	-2.254729	-1.269766
21	6	0	-1.196284	-3.780404	-1.474326

22	6	0	-3.558604	-3.486895	-1.922630
23	6	0	-2.335933	-1.818187	-0.748381
24	6	0	-1.146364	-2.539309	-0.834411
25	6	0	-2.391970	-4.243204	-2.020057
26	1	0	-4.477982	-3.868294	-2.354789
27	1	0	-2.415639	-5.203641	-2.524762
28	1	0	-0.295938	-4.381194	-1.557566
29	15	0	-0.729115	1.852443	-0.149976
30	15	0	0.365246	-1.742871	-0.137723
31	6	0	1.585997	-3.080244	-0.445234
32	6	0	3.424036	-5.093436	-1.077096
33	6	0	2.218166	-3.097607	-1.693901
34	6	0	1.884481	-4.079268	0.483912
35	6	0	2.806351	-5.077008	0.170524
36	6	0	3.125074	-4.104007	-2.012819
37	1	0	2.007547	-2.305840	-2.410962
38	1	0	1.399208	-4.078028	1.456076
39	1	0	3.038348	-5.844170	0.903084
40	1	0	3.608687	-4.108438	-2.984995
41	1	0	4.140575	-5.872415	-1.318990
42	6	0	0.050282	-1.864698	1.671811
43	6	0	-0.316818	-1.950437	4.444906
44	6	0	-0.946370	-2.671587	2.228241
45	6	0	0.858776	-1.095588	2.518143
46	6	0	0.680834	-1.146605	3.897614
47	6	0	-1.131754	-2.709436	3.608715
48	1	0	-1.580338	-3.275065	1.584025
49	1	0	1.617644	-0.444002	2.087819
50	1	0	1.309107	-0.540173	4.542590
51	1	0	-1.911482	-3.336974	4.030108
52	1	0	-0.463316	-1.979899	5.520545
53	6	0	-0.453787	3.619042	-0.564483
54	6	0	-0.020254	6.267054	-1.354089
55	6	0	-0.815025	4.674620	0.278380
56	6	0	0.124112	3.902550	-1.805722
57	6	0	0.333764	5.220136	-2.203157
58	6	0	-0.592951	5.992981	-0.113650
59	1	0	-1.266981	4.465585	1.244421
60	1	0	0.433061	3.079827	-2.447440
61	1	0	0.786889	5.428290	-3.167577
62	1	0	-0.869202	6.807028	0.549590
63	1	0	0.153735	7.295219	-1.656532
64	6	0	-0.846903	1.875995	1.687789
65	6	0	-0.830089	1.843574	4.489117
66	6	0	-1.945604	1.385638	2.395251
67	6	0	0.270419	2.334876	2.399611
68	6	0	0.272141	2.334227	3.789728
69	6	0	-1.931821	1.362632	3.789525
70	1	0	-2.820697	1.021136	1.865615
71	1	0	1.143846	2.689599	1.856528
72	1	0	1.139888	2.705107	4.327536
73	1	0	-2.789449	0.969148	4.327013
74	1	0	-0.824911	1.829418	5.574981
75	28	0	1.049962	0.431988	-0.495798
76	6	0	4.018909	-0.681300	-0.132301
77	1	0	3.701545	-1.336389	0.693745
78	1	0	4.048014	-1.325477	-1.018840

79	6	0	2.971713	0.371707	-0.317745
80	6	0	2.600732	1.592829	-0.373494
81	7	0	5.387819	-0.257654	0.144400
82	6	0	6.146404	0.140114	-1.033885
83	1	0	6.178917	-0.715479	-1.720851
84	1	0	7.177829	0.322727	-0.699818
85	6	0	5.654178	1.350238	-1.789804
86	1	0	5.562089	2.276940	-1.223742
87	6	0	5.360561	1.343535	-3.087337
88	1	0	5.026488	2.236941	-3.606922
89	1	0	5.440717	0.433128	-3.678224
90	6	0	5.487768	0.666423	1.255523
91	1	0	4.994969	0.226012	2.129687
92	1	0	5.020659	1.646677	1.072244
93	1	0	6.543224	0.825695	1.502209
94	1	0	3.066409	3.382612	-1.434511
95	1	0	3.939669	3.216629	0.095424
96	6	0	2.977063	3.032977	-0.398171
97	1	0	2.225627	3.670790	0.079632

Zero-point correction= 0.800492
(Hartree/Particle)
Thermal correction to Energy= 0.849179
Thermal correction to Enthalpy= 0.850123
Thermal correction to Gibbs Free Energy= 0.716666
Sum of electronic and zero-point Energies= -2798.315608
Sum of electronic and thermal Energies= -2798.266922
Sum of electronic and thermal Enthalpies= -2798.265978
Sum of electronic and thermal Free Energies= -2798.399435

XIa



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.003103	0.650998	-0.284352
2	5	0	0.086064	-0.949767	-1.575651
3	8	0	0.046145	-0.933761	-2.965653
4	6	0	0.264462	-2.266887	-3.476782
5	6	0	-0.020158	-3.170768	-2.231365
6	8	0	0.175485	-2.267387	-1.130446
7	6	0	-1.462234	-3.669916	-2.159695
8	1	0	-1.657792	-4.439055	-2.914689
9	1	0	-2.172876	-2.852375	-2.300522
10	1	0	-1.633031	-4.101786	-1.167942
11	6	0	0.934832	-4.347138	-2.067009
12	1	0	0.889626	-5.012853	-2.936214
13	1	0	0.650198	-4.925142	-1.182163

14	1	0	1.964677	-4.007331	-1.934956
15	6	0	-0.669992	-2.497136	-4.656766
16	1	0	-0.570721	-3.521394	-5.033579
17	1	0	-0.407120	-1.809405	-5.466796
18	1	0	-1.712167	-2.322349	-4.382277
19	6	0	1.711972	-2.355219	-3.948257
20	1	0	1.916359	-3.324323	-4.415860
21	1	0	2.408206	-2.211439	-3.118181
22	1	0	1.895620	-1.567650	-4.684632
23	6	0	-0.107072	2.120822	1.071072
24	6	0	-0.081254	1.867019	2.392912
25	1	0	0.038639	0.838773	2.746206
26	6	0	-0.195375	2.907722	3.487951
27	1	0	-1.074698	3.552293	3.347295
28	1	0	0.678248	3.576690	3.506300
29	1	0	-0.276374	2.445885	4.476602
30	6	0	-0.313547	3.582261	0.678686
31	1	0	0.364623	4.223886	1.263125
32	1	0	-1.335808	3.881353	0.966369
33	7	0	-0.140622	3.978239	-0.719881
34	6	0	1.229829	3.845813	-1.171536
35	1	0	1.528582	2.787270	-1.277568
36	1	0	1.908881	4.316080	-0.452530
37	1	0	1.352810	4.330856	-2.144688
38	6	0	-1.058098	3.320738	-1.626652
39	1	0	-0.706106	2.299753	-1.900677
40	1	0	-2.015376	3.177445	-1.107364
41	6	0	-1.322683	4.087075	-2.897919
42	1	0	-1.845037	3.527080	-3.674067
43	6	0	-0.986981	5.356097	-3.109897
44	1	0	-1.220432	5.857965	-4.043605
45	1	0	-0.471119	5.924164	-2.341106
46	1	0	4.670048	-1.854182	3.790874
47	6	0	3.720133	-1.759298	3.275601
48	6	0	1.287759	-1.491951	1.988853
49	6	0	2.619693	-2.503809	3.698039
50	6	0	3.601481	-0.904889	2.187179
51	6	0	2.382058	-0.757559	1.514074
52	6	0	1.390992	-2.395112	3.053428
53	1	0	2.730463	-3.182721	4.537083
54	1	0	4.458971	-0.322835	1.859991
55	6	0	0.182167	-3.277288	3.338865
56	8	0	0.084177	-1.302730	1.375200
57	6	0	0.168334	-4.393155	2.266090
58	1	0	1.076191	-5.001019	2.345201
59	1	0	0.125185	-3.959575	1.260582
60	1	0	-0.705929	-5.037904	2.407676
61	6	0	0.237456	-3.912856	4.726562
62	1	0	0.249016	-3.156131	5.517709
63	1	0	1.129325	-4.537573	4.825089
64	1	0	-0.622917	-4.569627	4.881008
65	6	0	-1.074262	-2.441395	3.129909
66	6	0	-3.393887	-1.060116	2.381019
67	6	0	-2.255008	-2.591375	3.851493
68	6	0	-1.073522	-1.545965	2.054592
69	6	0	-2.226825	-0.873732	1.630360
70	6	0	-3.408090	-1.896583	3.490364

71	1	0	-2.284730	-3.262158	4.703668
72	1	0	-4.319319	-2.018817	4.066276
73	1	0	-4.294727	-0.521933	2.099510
74	15	0	2.217811	0.390635	0.086295
75	15	0	-2.198359	0.206327	0.140769
76	6	0	-3.376515	1.544352	0.631722
77	6	0	-5.005756	3.723924	1.320288
78	6	0	-3.315747	2.103345	1.915114
79	6	0	-4.278837	2.080162	-0.293026
80	6	0	-5.084163	3.166063	0.048444
81	6	0	-4.124567	3.182943	2.255527
82	1	0	-2.626134	1.695850	2.646815
83	1	0	-4.357471	1.655269	-1.289592
84	1	0	-5.774551	3.571821	-0.684427
85	1	0	-4.061781	3.603638	3.254782
86	1	0	-5.630040	4.571610	1.584835
87	6	0	-3.216815	-0.689276	-1.104729
88	6	0	-4.751150	-1.848871	-3.140821
89	6	0	-4.170614	-1.665426	-0.802502
90	6	0	-3.031687	-0.308709	-2.439131
91	6	0	-3.807562	-0.871943	-3.450179
92	6	0	-4.925276	-2.248887	-1.817262
93	1	0	-4.316451	-1.990959	0.222441
94	1	0	-2.256682	0.412948	-2.687760
95	1	0	-3.657142	-0.562310	-4.480120
96	1	0	-5.651473	-3.018318	-1.573226
97	1	0	-5.343831	-2.302887	-3.929092
98	6	0	3.277139	1.803955	0.647552
99	6	0	4.678564	4.095727	1.472359
100	6	0	3.104975	2.322504	1.938915
101	6	0	4.181582	2.435666	-0.210729
102	6	0	4.874293	3.574858	0.197709
103	6	0	3.797856	3.458586	2.345157
104	1	0	2.421718	1.838217	2.627666
105	1	0	4.353200	2.049714	-1.209886
106	1	0	5.569154	4.051035	-0.487346
107	1	0	3.649796	3.845074	3.349257
108	1	0	5.215265	4.985027	1.788394
109	6	0	3.276532	-0.310688	-1.242869
110	6	0	4.970353	-1.044170	-3.349404
111	6	0	4.206246	-1.339575	-1.073740
112	6	0	3.171504	0.313268	-2.493471
113	6	0	4.033858	-0.028394	-3.530218
114	6	0	5.038313	-1.712789	-2.129250
115	1	0	4.284823	-1.854061	-0.120856
116	1	0	2.407792	1.071973	-2.652730
117	1	0	3.953399	0.477964	-4.487306
118	1	0	5.752268	-2.518837	-1.990270
119	1	0	5.633155	-1.325035	-4.161999

Zero-point correction= 0.998082
(Hartree/Particle)
Thermal correction to Energy= 1.056391
Thermal correction to Enthalpy= 1.057335
Thermal correction to Gibbs Free Energy= 0.907816
Sum of electronic and zero-point Energies= -3209.814714
Sum of electronic and thermal Energies= -3209.756406

Sum of electronic and thermal Enthalpies= -3209.755462
Sum of electronic and thermal Free Energies= -3209.904980

$TS_{Xa\text{-}XIa}$

Imaginary frequency: -956.1779

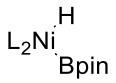
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.013159	1.023190	1.536136
2	5	0	-1.610305	-0.102086	1.867527
3	8	0	-2.736939	0.266752	2.585730
4	6	0	-3.769960	-0.710801	2.336803
5	6	0	-2.942017	-1.963052	1.914950
6	8	0	-1.771687	-1.365318	1.321651
7	6	0	-2.457929	-2.788815	3.107194
8	1	0	-3.280719	-3.325040	3.590609
9	1	0	-1.973034	-2.145350	3.850507
10	1	0	-1.721572	-3.516805	2.752280
11	6	0	-3.613519	-2.861316	0.889597
12	1	0	-4.542614	-3.280132	1.293560
13	1	0	-2.941220	-3.685498	0.630473
14	1	0	-3.840780	-2.311342	-0.027811
15	6	0	-4.597222	-0.887934	3.600261
16	1	0	-5.332514	-1.689808	3.469358
17	1	0	-5.137316	0.038419	3.817257
18	1	0	-3.966994	-1.126143	4.459715
19	6	0	-4.636379	-0.175528	1.200892
20	1	0	-5.493175	-0.828993	1.005802
21	1	0	-4.050211	-0.081887	0.282402
22	1	0	-5.006974	0.817359	1.473224
23	6	0	1.628856	1.864544	2.267534
24	6	0	1.219086	1.042780	3.157866
25	1	0	-0.127747	0.239965	2.849562
26	6	0	1.476375	0.455102	4.501466
27	1	0	2.313718	0.978689	4.975315
28	1	0	1.738138	-0.605631	4.419037
29	1	0	0.599738	0.535927	5.152090
30	6	0	2.809193	2.783261	2.099462
31	1	0	3.152047	3.118395	3.089062
32	1	0	2.530344	3.674709	1.528009
33	7	0	3.952850	2.169261	1.427977
34	6	0	4.403106	0.970097	2.116784
35	1	0	3.647705	0.162890	2.103703
36	1	0	4.627102	1.209344	3.162347
37	1	0	5.317777	0.601307	1.644295
38	6	0	3.695643	1.914100	0.018208
39	1	0	3.075587	1.010727	-0.131330
40	1	0	3.097214	2.743156	-0.379820
41	6	0	4.946822	1.813298	-0.812615
42	1	0	4.788599	1.452182	-1.827882
43	6	0	6.170060	2.147888	-0.409222
44	1	0	7.026404	2.073488	-1.072689
45	1	0	6.340292	2.518666	0.597674
46	1	0	-1.001359	-5.859522	-1.202022
47	6	0	-0.985178	-4.777780	-1.288664
48	6	0	-0.962065	-2.031623	-1.491240

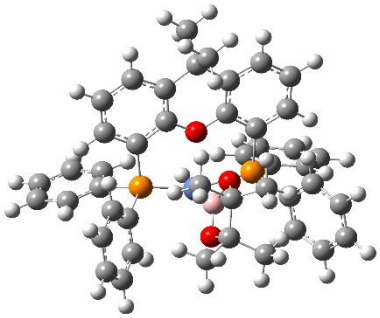
49	6	0	-1.952278	-4.128452	-2.051274
50	6	0	0.013947	-4.043567	-0.654725
51	6	0	0.042960	-2.651990	-0.748102
52	6	0	-1.949263	-2.739124	-2.176866
53	1	0	-2.712776	-4.714516	-2.556322
54	1	0	0.778238	-4.554309	-0.076233
55	6	0	-2.884413	-1.951250	-3.082657
56	8	0	-0.919188	-0.656175	-1.560593
57	6	0	-2.136387	-1.677475	-4.408199
58	1	0	-1.892375	-2.623301	-4.903635
59	1	0	-1.204804	-1.132638	-4.222590
60	1	0	-2.760525	-1.075617	-5.077062
61	6	0	-4.172349	-2.716161	-3.388844
62	1	0	-4.740105	-2.931783	-2.477557
63	1	0	-3.944471	-3.660352	-3.890424
64	1	0	-4.807255	-2.145869	-4.071906
65	6	0	-3.153377	-0.604395	-2.420309
66	6	0	-3.398201	1.992394	-1.403966
67	6	0	-4.352829	0.094706	-2.543178
68	6	0	-2.099225	0.017444	-1.741195
69	6	0	-2.175811	1.328718	-1.249654
70	6	0	-4.478075	1.381646	-2.032705
71	1	0	-5.196926	-0.362720	-3.047536
72	1	0	-5.418994	1.913965	-2.124881
73	1	0	-3.524984	2.989139	-1.000997
74	15	0	1.339241	-1.580118	0.011437
75	15	0	-0.762714	2.059173	-0.291689
76	6	0	-1.447879	3.685072	0.215012
77	6	0	-2.495085	6.124839	1.104894
78	6	0	-1.605233	3.932122	1.581335
79	6	0	-1.825083	4.675761	-0.703274
80	6	0	-2.343723	5.887832	-0.262049
81	6	0	-2.128163	5.147640	2.023876
82	1	0	-1.315797	3.168455	2.299525
83	1	0	-1.709114	4.494867	-1.769569
84	1	0	-2.629937	6.647645	-0.982740
85	1	0	-2.245013	5.326944	3.088025
86	1	0	-2.898148	7.072041	1.449927
87	6	0	0.523191	2.506350	-1.543238
88	6	0	2.690484	3.077945	-3.244037
89	6	0	1.127546	1.494244	-2.302135
90	6	0	1.041388	3.804470	-1.632920
91	6	0	2.107081	4.088551	-2.486540
92	6	0	2.201174	1.776887	-3.141379
93	1	0	0.773929	0.473061	-2.227700
94	1	0	0.630361	4.603732	-1.026338
95	1	0	2.490088	5.102955	-2.542372
96	1	0	2.663626	0.967163	-3.700573
97	1	0	3.531202	3.298479	-3.894751
98	6	0	1.955957	-2.714987	1.326241
99	6	0	2.662997	-4.381108	3.469052
100	6	0	1.252553	-2.660155	2.536857
101	6	0	3.018285	-3.615799	1.202924
102	6	0	3.371539	-4.439495	2.271364
103	6	0	1.596641	-3.492820	3.597911
104	1	0	0.419900	-1.967040	2.632885
105	1	0	3.570697	-3.680486	0.269732

106	1	0	4.199431	-5.133866	2.163354
107	1	0	1.034263	-3.443459	4.526370
108	1	0	2.939772	-5.025200	4.298032
109	6	0	2.642165	-1.713594	-1.293269
110	6	0	4.643558	-1.646870	-3.270794
111	6	0	2.341621	-2.012529	-2.628133
112	6	0	3.963539	-1.373241	-0.970215
113	6	0	4.956488	-1.351621	-1.945147
114	6	0	3.332799	-1.974988	-3.607993
115	1	0	1.328438	-2.286272	-2.910418
116	1	0	4.222318	-1.122621	0.056802
117	1	0	5.970924	-1.082055	-1.666642
118	1	0	3.078111	-2.212151	-4.636877
119	1	0	5.415678	-1.622229	-4.033714

Zero-point correction= 0.992680
(Hartree/Particle)
Thermal correction to Energy= 1.051511
Thermal correction to Enthalpy= 1.052455
Thermal correction to Gibbs Free Energy= 0.899092
Sum of electronic and zero-point Energies= -3209.778252
Sum of electronic and thermal Energies= -3209.719422
Sum of electronic and thermal Enthalpies= -3209.718478
Sum of electronic and thermal Free Energies= -3209.871840

XII





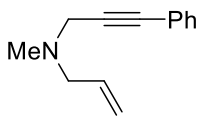
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.666022	2.427782	-2.864583
2	6	0	-3.690287	2.177687	-2.461949
3	6	0	-1.192925	1.571703	-1.434726
4	6	0	-2.537723	2.518369	-3.160404
5	6	0	-3.583882	1.518407	-1.241285
6	6	0	-2.336182	1.182733	-0.715959
7	6	0	-1.265610	2.232734	-2.661149
8	1	0	-2.628651	3.032370	-4.113669
9	1	0	-4.481886	1.256798	-0.687609
10	6	0	-0.013769	2.644923	-3.430787
11	8	0	0.000413	1.297820	-0.846840

12	6	0	-0.013707	1.946645	-4.804400
13	1	0	-0.897514	2.232213	-5.383418
14	1	0	-0.016614	0.859500	-4.682203
15	1	0	0.871936	2.228982	-5.382248
16	6	0	-0.022565	4.173636	-3.627171
17	1	0	-0.019045	4.685857	-2.660718
18	1	0	-0.912250	4.487221	-4.181640
19	1	0	0.855998	4.497059	-4.193663
20	6	0	1.246506	2.245491	-2.667853
21	6	0	3.579334	1.579415	-1.246933
22	6	0	2.512476	2.557943	-3.165958
23	6	0	1.186946	1.576586	-1.444005
24	6	0	2.339494	1.197131	-0.731516
25	6	0	3.671603	2.247213	-2.463908
26	1	0	2.592771	3.078444	-4.116642
27	1	0	4.640925	2.531893	-2.858892
28	1	0	4.481078	1.356517	-0.682224
29	15	0	-2.185006	0.277243	0.887215
30	15	0	2.200888	0.266884	0.859482
31	6	0	3.346685	1.241987	1.934381
32	6	0	5.026160	2.851115	3.492762
33	6	0	2.843967	2.380084	2.572393
34	6	0	4.696937	0.911254	2.092460
35	6	0	5.530997	1.713104	2.869920
36	6	0	3.681343	3.182925	3.341406
37	1	0	1.787506	2.613909	2.472711
38	1	0	5.102916	0.023623	1.615694
39	1	0	6.576052	1.443758	2.989643
40	1	0	3.278945	4.064542	3.831198
41	1	0	5.676223	3.473456	4.100221
42	6	0	3.190136	-1.267625	0.624042
43	6	0	4.704455	-3.625874	0.578954
44	6	0	4.036774	-1.543828	-0.451535
45	6	0	3.092410	-2.199227	1.665470
46	6	0	3.851208	-3.363424	1.650373
47	6	0	4.786361	-2.721515	-0.475367
48	1	0	4.111715	-0.852110	-1.284442
49	1	0	2.403031	-2.013001	2.485834
50	1	0	3.765833	-4.073351	2.467052
51	1	0	5.436893	-2.925997	-1.320377
52	1	0	5.293812	-4.537473	0.561873
53	6	0	-3.327141	1.253780	1.963935
54	6	0	-5.003318	2.864422	3.525917
55	6	0	-4.700793	0.990578	2.033957
56	6	0	-2.801878	2.325137	2.691629
57	6	0	-3.637350	3.128542	3.463847
58	6	0	-5.532937	1.792434	2.811528
59	1	0	-5.126390	0.153254	1.487403
60	1	0	-1.731345	2.508378	2.655808
61	1	0	-3.216226	3.957076	4.025442
62	1	0	-6.595794	1.575818	2.860226
63	1	0	-5.652134	3.486905	4.134552
64	6	0	-3.184275	-1.249997	0.649478
65	6	0	-4.708092	-3.597857	0.514001
66	6	0	-3.776072	-1.637598	-0.553767
67	6	0	-3.337866	-2.066612	1.777461
68	6	0	-4.098849	-3.229042	1.713014

69	6	0	-4.538223	-2.805717	-0.617585
70	1	0	-3.637479	-1.037368	-1.447574
71	1	0	-2.863377	-1.785147	2.715510
72	1	0	-4.211373	-3.848991	2.597044
73	1	0	-4.995012	-3.096061	-1.559342
74	1	0	-5.302530	-4.504661	0.461620
75	28	0	0.005099	0.142009	1.303903
76	1	0	0.025369	1.454746	2.192943
77	5	0	-0.042297	-1.484387	0.111011
78	8	0	-0.465345	-1.449789	-1.213638
79	8	0	0.362798	-2.758935	0.454545
80	6	0	-0.101494	-2.689212	-1.849830
81	6	0	0.087721	-3.660214	-0.635005
82	6	0	1.260942	-4.619989	-0.770229
83	1	0	2.205603	-4.079056	-0.870138
84	1	0	1.128850	-5.276299	-1.638219
85	1	0	1.324114	-5.244151	0.126538
86	6	0	-1.185221	-4.418427	-0.271987
87	1	0	-2.022284	-3.726073	-0.148927
88	1	0	-1.028630	-4.934552	0.679978
89	1	0	-1.446546	-5.160577	-1.033810
90	6	0	1.192449	-2.419159	-2.616515
91	1	0	1.019265	-1.596754	-3.317630
92	1	0	1.524021	-3.296937	-3.180750
93	1	0	1.990226	-2.120753	-1.930494
94	6	0	-1.202886	-3.090039	-2.820783
95	1	0	-1.283448	-2.334849	-3.609221
96	1	0	-2.169360	-3.165589	-2.317671
97	1	0	-0.972758	-4.053080	-3.290425

Zero-point correction=	0.795102
(Hartree/Particle)	
Thermal correction to Energy=	0.842913
Thermal correction to Enthalpy=	0.843857
Thermal correction to Gibbs Free Energy=	0.713308
Sum of electronic and zero-point Energies=	-2842.801724
Sum of electronic and thermal Energies=	-2842.753913
Sum of electronic and thermal Enthalpies=	-2842.752969
Sum of electronic and thermal Free Energies=	-2842.883518

Enyne-Ph (B)

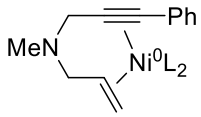


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.983706	-0.510363	-0.430397
2	6	0	-4.248585	-1.167535	-0.728673
3	1	0	-4.793415	-1.481175	0.181219
4	1	0	-4.069016	-2.051282	-1.347090
5	1	0	-4.889760	-0.482000	-1.289545
6	6	0	-3.251741	0.718094	0.324349

7	1	0	-3.774741	0.470367	1.271382
8	1	0	-3.942016	1.320213	-0.276712
9	6	0	-2.112277	-1.433210	0.295794
10	1	0	-2.405465	-1.516476	1.360580
11	1	0	-2.244200	-2.430799	-0.137791
12	6	0	-0.687545	-1.088010	0.202140
13	6	0	0.487418	-0.815401	0.125381
14	6	0	-2.040159	1.551327	0.644424
15	1	0	-1.342033	1.154966	1.378146
16	6	0	-1.819160	2.748568	0.108842
17	1	0	-0.954685	3.345498	0.383418
18	1	0	-2.498867	3.174436	-0.625428
19	6	0	1.865525	-0.430926	0.020558
20	6	0	4.542298	0.345932	-0.192738
21	6	0	2.193951	0.880807	-0.351272
22	6	0	2.891034	-1.348513	0.285636
23	6	0	4.221176	-0.958318	0.178677
24	6	0	3.526097	1.262989	-0.457113
25	1	0	1.393613	1.585689	-0.554961
26	1	0	2.634203	-2.363308	0.571768
27	1	0	5.009737	-1.675535	0.383856
28	1	0	3.772606	2.279930	-0.746021
29	1	0	5.581791	0.647188	-0.276065

Zero-point correction= 0.249187
(Hartree/Particle)
Thermal correction to Energy= 0.262944
Thermal correction to Enthalpy= 0.263888
Thermal correction to Gibbs Free Energy= 0.205940
Sum of electronic and zero-point Energies= -558.551173
Sum of electronic and thermal Energies= -558.537416
Sum of electronic and thermal Enthalpies= -558.536472
Sum of electronic and thermal Free Energies= -558.594420

IIb



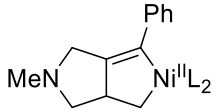
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.072101	1.635475	-0.863502
2	6	0	1.260479	2.256519	-3.700107
3	1	0	1.858476	1.616642	-4.361382
4	1	0	0.499825	2.753607	-4.338172
5	6	0	0.540862	1.432002	-2.701712
6	6	0	-0.228925	0.457725	-2.437149
7	7	0	2.150099	3.254441	-3.111556
8	6	0	1.487425	4.026106	-2.065612
9	1	0	0.500483	4.412566	-2.389452
10	1	0	2.125925	4.897575	-1.868022
11	6	0	1.360648	3.246482	-0.787395
12	1	0	2.281206	2.743563	-0.494594

13	6	0	0.384266	3.419932	0.163776
14	1	0	0.563711	3.112637	1.189894
15	1	0	-0.451868	4.098463	-0.005557
16	6	0	2.672339	4.115058	-4.157510
17	1	0	3.182071	3.506586	-4.911113
18	1	0	3.395585	4.818502	-3.735907
19	1	0	1.878955	4.693412	-4.667845
20	1	0	-5.439652	-2.209916	-0.424236
21	6	0	-4.383229	-2.076606	-0.213729
22	6	0	-1.709330	-1.747216	0.317970
23	6	0	-3.520786	-3.167475	-0.287297
24	6	0	-3.897682	-0.813873	0.113498
25	6	0	-2.539216	-0.625092	0.378632
26	6	0	-2.161439	-3.024041	-0.011973
27	1	0	-3.916595	-4.140430	-0.560009
28	1	0	-4.575011	0.033777	0.139334
29	6	0	-1.159438	-4.171545	0.048394
30	8	0	-0.386458	-1.542332	0.630458
31	6	0	-1.022822	-4.599886	1.528231
32	1	0	-1.985367	-4.958276	1.908403
33	1	0	-0.696605	-3.757770	2.148447
34	1	0	-0.283256	-5.402554	1.620661
35	6	0	-1.608041	-5.374756	-0.780378
36	1	0	-1.731548	-5.105061	-1.833899
37	1	0	-2.556232	-5.767725	-0.402930
38	1	0	-0.878903	-6.186134	-0.702389
39	6	0	0.196374	-3.633699	-0.395199
40	6	0	2.753452	-2.551801	-0.858830
41	6	0	1.163784	-4.362717	-1.086283
42	6	0	0.537292	-2.340706	-0.002785
43	6	0	1.804580	-1.783314	-0.181195
44	6	0	2.424973	-3.821850	-1.329801
45	1	0	0.938524	-5.364933	-1.436126
46	1	0	3.165750	-4.404733	-1.867909
47	1	0	3.749528	-2.151809	-1.022726
48	15	0	-1.739819	1.018051	0.601427
49	15	0	2.054900	-0.082111	0.474169
50	6	0	3.815138	0.188180	0.008288
51	6	0	6.427326	0.660693	-0.882362
52	6	0	4.043815	0.793431	-1.234528
53	6	0	4.908982	-0.174181	0.801818
54	6	0	6.207778	0.063384	0.358064
55	6	0	5.343516	1.024498	-1.678775
56	1	0	3.199376	1.099488	-1.850481
57	1	0	4.743960	-0.642024	1.768857
58	1	0	7.051073	-0.219607	0.981056
59	1	0	5.504755	1.499447	-2.641964
60	1	0	7.441286	0.845870	-1.224168
61	6	0	2.183097	-0.395935	2.285165
62	6	0	2.383375	-0.649019	5.070792
63	6	0	2.126310	-1.655226	2.888428
64	6	0	2.321809	0.736472	3.098418
65	6	0	2.435120	0.611928	4.478367
66	6	0	2.220144	-1.779093	4.274308
67	1	0	2.020788	-2.546909	2.275556
68	1	0	2.343424	1.725294	2.642914
69	1	0	2.543430	1.500509	5.093297

70	1	0	2.175113	-2.764303	4.729743
71	1	0	2.461049	-0.748511	6.149522
72	6	0	-3.163633	2.163713	0.406657
73	6	0	-5.307274	3.904888	-0.044919
74	6	0	-4.148000	2.343262	1.386329
75	6	0	-3.263904	2.867868	-0.797749
76	6	0	-4.333109	3.732764	-1.024612
77	6	0	-5.213392	3.209916	1.160871
78	1	0	-4.075120	1.804919	2.328052
79	1	0	-2.492439	2.737689	-1.555037
80	1	0	-4.400100	4.275195	-1.962679
81	1	0	-5.971229	3.344725	1.926450
82	1	0	-6.137391	4.583167	-0.217161
83	6	0	-1.421268	1.103051	2.413737
84	6	0	-0.811858	1.347006	5.140641
85	6	0	-1.240975	-0.034781	3.205969
86	6	0	-1.288807	2.365896	3.006988
87	6	0	-0.988679	2.487301	4.360632
88	6	0	-0.939298	0.088748	4.559912
89	1	0	-1.336064	-1.024656	2.772645
90	1	0	-1.446068	3.262483	2.411692
91	1	0	-0.897473	3.473853	4.805052
92	1	0	-0.792997	-0.805443	5.158158
93	1	0	-0.572396	1.438883	6.195962
94	1	0	-0.347118	-3.925705	-3.909258
95	6	0	-0.910078	-3.033873	-3.646401
96	6	0	-2.332942	-0.754607	-2.930646
97	6	0	-2.300072	-3.029053	-3.740872
98	6	0	-0.228873	-1.900549	-3.211582
99	6	0	-0.930920	-0.739630	-2.857977
100	6	0	-3.008198	-1.883086	-3.377749
101	1	0	-2.829364	-3.913493	-4.084170
102	1	0	0.854781	-1.911784	-3.124043
103	1	0	-4.093111	-1.873998	-3.429170
104	1	0	-2.883722	0.132836	-2.628495

Zero-point correction= 0.854146
(Hartree/Particle)
Thermal correction to Energy= 0.905152
Thermal correction to Enthalpy= 0.906096
Thermal correction to Gibbs Free Energy= 0.769582
Sum of electronic and zero-point Energies= -2989.945098
Sum of electronic and thermal Energies= -2989.894092
Sum of electronic and thermal Enthalpies= -2989.893148
Sum of electronic and thermal Free Energies= -2990.029662

IIIb



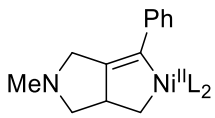
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-6.457289	0.380736	-0.343273
2	6	0	-5.440934	0.057252	-0.542978
3	6	0	-2.871141	-0.776930	-1.019946
4	6	0	-5.217054	-1.151070	-1.205119
5	6	0	-4.372388	0.848363	-0.137527
6	6	0	-3.053292	0.441729	-0.374836
7	6	0	-3.921066	-1.587982	-1.460284
8	1	0	-6.065107	-1.752839	-1.515251
9	1	0	-4.559781	1.778325	0.391704
10	6	0	-3.537582	-2.866920	-2.202209
11	8	0	-1.576130	-1.211067	-1.204432
12	6	0	-4.705080	-3.846583	-2.302882
13	1	0	-5.533290	-3.394019	-2.855555
14	1	0	-5.067030	-4.148574	-1.314745
15	1	0	-4.404870	-4.741903	-2.854772
16	6	0	-3.073212	-2.489974	-3.626779
17	1	0	-2.234582	-1.789060	-3.597575
18	1	0	-3.896990	-2.021998	-4.175083
19	1	0	-2.756813	-3.389107	-4.165330
20	6	0	-2.357784	-3.456063	-1.435865
21	6	0	-0.157532	-4.296759	0.095585
22	6	0	-2.168687	-4.804817	-1.147773
23	6	0	-1.402618	-2.554957	-0.958660
24	6	0	-0.315512	-2.931229	-0.172776
25	6	0	-1.067245	-5.223971	-0.401167
26	1	0	-2.888077	-5.539152	-1.495106
27	1	0	-0.933612	-6.278467	-0.183332
28	1	0	0.668120	-4.629435	0.716122
29	15	0	-1.565188	1.462464	0.030338
30	15	0	0.667266	-1.587785	0.612128
31	6	0	2.199683	-2.480021	1.104598
32	6	0	4.596909	-3.778938	1.755253
33	6	0	2.823731	-3.327878	0.182248
34	6	0	2.800541	-2.277455	2.350259
35	6	0	3.994911	-2.920260	2.669682
36	6	0	4.005992	-3.981276	0.510266
37	1	0	2.387559	-3.478562	-0.800713
38	1	0	2.336973	-1.627501	3.085150
39	1	0	4.447530	-2.754683	3.642597
40	1	0	4.474408	-4.634119	-0.219749
41	1	0	5.523505	-4.284860	2.008609
42	6	0	-0.217883	-1.373414	2.220692
43	6	0	-1.457707	-0.914679	4.693940
44	6	0	-1.265662	-2.193261	2.649866
45	6	0	0.178952	-0.298875	3.032047
46	6	0	-0.424482	-0.082272	4.267373
47	6	0	-1.884617	-1.959282	3.877999
48	1	0	-1.600414	-3.020950	2.031682
49	1	0	0.964055	0.375293	2.692457
50	1	0	-0.103141	0.751690	4.883393
51	1	0	-2.697527	-2.603508	4.198898
52	1	0	-1.935530	-0.742159	5.653630
53	6	0	-1.622006	2.640958	-1.385876
54	6	0	-1.668520	4.302609	-3.638659
55	6	0	-2.727735	3.461891	-1.639717
56	6	0	-0.545522	2.655963	-2.277510
57	6	0	-0.571146	3.481841	-3.400958

58	6	0	-2.747586	4.293185	-2.754884
59	1	0	-3.577038	3.456364	-0.961497
60	1	0	0.325667	2.031376	-2.088186
61	1	0	0.273909	3.484729	-4.082334
62	1	0	-3.607241	4.930605	-2.937728
63	1	0	-1.686075	4.949510	-4.510321
64	6	0	-2.205855	2.394403	1.473190
65	6	0	-3.070575	3.662360	3.814649
66	6	0	-2.650380	1.641210	2.566500
67	6	0	-2.195706	3.788766	1.565868
68	6	0	-2.627950	4.417878	2.732533
69	6	0	-3.080256	2.271012	3.729276
70	1	0	-2.660078	0.553905	2.508897
71	1	0	-1.854052	4.387971	0.726828
72	1	0	-2.616432	5.501698	2.792395
73	1	0	-3.415002	1.671043	4.570446
74	1	0	-3.405115	4.155222	4.722342
75	28	0	0.780506	0.811360	0.049677
76	1	0	1.528673	2.531707	1.605198
77	6	0	1.129806	2.693312	0.590838
78	1	0	0.272346	3.370780	0.679068
79	6	0	2.211049	3.259650	-0.310802
80	6	0	3.238247	4.285522	0.175891
81	7	0	4.301904	4.142598	-0.822304
82	6	0	4.468037	2.698501	-1.051968
83	6	0	3.103810	2.126207	-0.712594
84	1	0	1.746798	3.684162	-1.215616
85	1	0	3.588937	4.012202	1.192934
86	1	0	2.879439	5.320590	0.202169
87	1	0	5.239334	2.275998	-0.381182
88	1	0	4.796672	2.503422	-2.081120
89	6	0	5.532244	4.808428	-0.465954
90	1	0	6.269160	4.687813	-1.267084
91	1	0	5.974746	4.410718	0.468213
92	1	0	5.350287	5.879511	-0.328336
93	6	0	2.637935	0.870654	-0.608008
94	6	0	3.488277	-0.248243	-1.072760
95	6	0	5.184573	-2.250785	-2.110675
96	6	0	3.117139	-1.003233	-2.196389
97	6	0	4.712345	-0.553899	-0.456617
98	6	0	5.551952	-1.535797	-0.970873
99	6	0	3.958178	-1.985550	-2.716181
100	1	0	2.162565	-0.790179	-2.674625
101	1	0	5.000704	-0.003176	0.435168
102	1	0	6.495587	-1.750013	-0.476051
103	1	0	3.656772	-2.542272	-3.599683
104	1	0	5.844135	-3.012671	-2.515980

Zero-point correction= 0.857302
(Hartree/Particle)
Thermal correction to Energy= 0.906957
Thermal correction to Enthalpy= 0.907901
Thermal correction to Gibbs Free Energy= 0.774533
Sum of electronic and zero-point Energies= -2989.941542
Sum of electronic and thermal Energies= -2989.891886
Sum of electronic and thermal Enthalpies= -2989.890942
Sum of electronic and thermal Free Energies= -2990.024311

IIIb-HBpin



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.916351	-0.483357	0.710394
2	1	0	1.604082	-2.905362	-4.782915
3	6	0	1.717664	-2.175980	-3.987440
4	6	0	2.005519	-0.338463	-1.964698
5	6	0	2.978691	-1.932126	-3.447363
6	6	0	0.601429	-1.493242	-3.512595
7	6	0	0.726405	-0.563574	-2.478075
8	6	0	3.147268	-0.992867	-2.429538
9	1	0	3.837070	-2.475338	-3.829685
10	1	0	-0.377982	-1.701440	-3.930723
11	6	0	4.484856	-0.578600	-1.827109
12	8	0	2.113556	0.585639	-0.948028
13	6	0	4.900408	0.766010	-2.468769
14	1	0	5.036351	0.641227	-3.548227
15	1	0	4.138265	1.533710	-2.300170
16	1	0	5.842218	1.114015	-2.031733
17	6	0	5.585816	-1.606888	-2.081359
18	1	0	5.345019	-2.580643	-1.642424
19	1	0	5.745958	-1.737399	-3.155309
20	1	0	6.533209	-1.259566	-1.659679
21	6	0	4.246725	-0.332581	-0.341534
22	6	0	3.704440	0.428005	2.310199
23	6	0	5.147389	-0.630361	0.681527
24	6	0	3.065203	0.314711	0.015382
25	6	0	2.765166	0.717855	1.318458
26	6	0	4.877046	-0.255139	1.995061
27	1	0	6.073065	-1.149314	0.454429
28	1	0	5.591636	-0.485563	2.778607
29	1	0	3.508448	0.723667	3.336257
30	15	0	-0.707254	0.247843	-1.653054
31	15	0	1.110161	1.478225	1.593249
32	6	0	1.203127	1.869649	3.385983
33	6	0	1.296500	2.277715	6.153613
34	6	0	0.914289	0.821133	4.269716
35	6	0	1.530715	3.125931	3.902839
36	6	0	1.571944	3.327849	5.281409
37	6	0	0.970768	1.021157	5.645780
38	1	0	0.648997	-0.157167	3.873280
39	1	0	1.752731	3.948719	3.229206
40	1	0	1.823520	4.308686	5.673712
41	1	0	0.750101	0.199388	6.320081
42	1	0	1.331027	2.438743	7.226736
43	6	0	1.323975	3.122449	0.803765
44	6	0	1.482882	5.685838	-0.307071

45	6	0	2.569538	3.709229	0.555929
46	6	0	0.160963	3.823675	0.468354
47	6	0	0.239465	5.104502	-0.070635
48	6	0	2.647041	4.983096	-0.002679
49	1	0	3.480334	3.171578	0.807313
50	1	0	-0.811513	3.359270	0.613135
51	1	0	-0.671654	5.635576	-0.328101
52	1	0	3.618428	5.430677	-0.191177
53	1	0	1.546263	6.680782	-0.737831
54	6	0	-2.121068	-0.519627	-2.536640
55	6	0	-4.302116	-1.794140	-3.736515
56	6	0	-2.582949	-1.746682	-2.042067
57	6	0	-2.743621	0.048101	-3.650869
58	6	0	-3.835582	-0.583139	-4.242642
59	6	0	-3.666433	-2.381469	-2.643389
60	1	0	-2.095030	-2.198346	-1.181435
61	1	0	-2.385651	0.991100	-4.052133
62	1	0	-4.320630	-0.126812	-5.100035
63	1	0	-4.023199	-3.327558	-2.247712
64	1	0	-5.156922	-2.281742	-4.195320
65	6	0	-0.651125	1.967589	-2.298976
66	6	0	-0.669817	4.617261	-3.211373
67	6	0	0.506368	2.540161	-2.834247
68	6	0	-1.815188	2.741753	-2.214041
69	6	0	-1.825607	4.054476	-2.674608
70	6	0	0.495006	3.858636	-3.283817
71	1	0	1.421691	1.963346	-2.913694
72	1	0	-2.727155	2.309507	-1.815845
73	1	0	-2.743633	4.631649	-2.607986
74	1	0	1.403148	4.290760	-3.692910
75	1	0	-0.674822	5.643778	-3.566144
76	7	0	-4.813740	-2.689086	2.666362
77	6	0	-4.888602	-1.440545	1.894804
78	6	0	-3.459395	-1.223249	1.444098
79	6	0	-2.586250	-2.280637	2.063449
80	6	0	-3.464979	-2.738787	3.234425
81	1	0	-5.220591	-0.590867	2.524679
82	1	0	-5.614162	-1.540639	1.077937
83	1	0	-3.353910	-2.026593	4.078566
84	1	0	-3.245901	-3.746473	3.606229
85	6	0	-5.864074	-2.814134	3.649853
86	1	0	-6.842153	-2.787439	3.157719
87	1	0	-5.836614	-2.002433	4.402429
88	1	0	-5.771654	-3.770770	4.174662
89	6	0	-2.844240	-0.208295	0.827663
90	6	0	-3.567976	0.973788	0.328837
91	6	0	-4.915047	3.275837	-0.592012
92	6	0	-4.553217	0.884366	-0.668538
93	6	0	-3.276623	2.244619	0.852079
94	6	0	-3.942298	3.381360	0.403439
95	6	0	-5.217021	2.022359	-1.123623
96	1	0	-4.778866	-0.089513	-1.097806
97	1	0	-2.521761	2.319883	1.632431
98	1	0	-3.701098	4.352244	0.828655
99	1	0	-5.969641	1.928277	-1.901668
100	1	0	-5.433215	4.161545	-0.947769
101	1	0	-2.473265	-3.129831	1.370352

102	6	0	-1.238082	-1.609573	2.316530
103	1	0	-0.439084	-2.315239	2.591913
104	1	0	-1.349185	-0.891393	3.140229
105	1	0	0.810502	-1.027838	0.515337
106	5	0	0.939778	-2.220224	0.475970
107	8	0	1.819057	-2.852574	1.299908
108	6	0	2.062704	-4.153421	0.707897
109	6	0	0.785191	-4.370956	-0.175026
110	8	0	0.385832	-3.010432	-0.484183
111	6	0	2.250035	-5.172826	1.818292
112	1	0	3.157607	-4.936005	2.380489
113	1	0	2.357357	-6.178433	1.398175
114	1	0	1.405600	-5.166690	2.510245
115	6	0	3.336256	-4.014499	-0.121542
116	1	0	4.140856	-3.649904	0.524526
117	1	0	3.187664	-3.287655	-0.927387
118	1	0	3.637309	-4.971147	-0.559881
119	6	0	-0.367496	-5.008060	0.594117
120	1	0	-0.553577	-4.479869	1.534933
121	1	0	-0.163473	-6.060333	0.813529
122	1	0	-1.274801	-4.948368	-0.014307
123	6	0	1.033283	-5.105288	-1.482168
124	1	0	1.726680	-4.551432	-2.119709
125	1	0	0.088180	-5.216390	-2.021826
126	1	0	1.440152	-6.103772	-1.289418

Zero-point correction=	1.052588
(Hartree/Particle)	
Thermal correction to Energy=	1.113320
Thermal correction to Enthalpy=	1.114265
Thermal correction to Gibbs Free Energy=	0.956529
Sum of electronic and zero-point Energies=	-3401.452251
Sum of electronic and thermal Energies=	-3401.391519
Sum of electronic and thermal Enthalpies=	-3401.390575
Sum of electronic and thermal Free Energies=	-3401.548310

$TS_{IIb\text{-}IIIb}$

imaginary frequencies = -152.6732 cm^{-1}

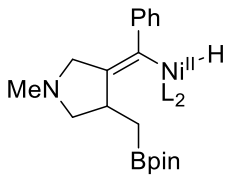
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.153588	-1.433476	-0.280921
2	1	0	-1.016372	-3.456736	1.156058
3	6	0	-0.260252	-3.263058	0.391808
4	1	0	0.695129	-3.745017	0.598213
5	6	0	-0.733250	-3.404010	-1.006931
6	6	0	-2.020477	-4.164519	-1.256689
7	7	0	-2.354991	-3.978031	-2.657449
8	6	0	-2.337053	-2.543745	-2.885432
9	6	0	-1.241476	-1.924162	-2.056364
10	1	0	0.047328	-3.782147	-1.671756
11	1	0	-2.816363	-3.791643	-0.578943
12	1	0	-1.876927	-5.231317	-1.053034
13	1	0	-3.304436	-2.092050	-2.576065
14	1	0	-2.203942	-2.315842	-3.949584

15	1	0	-3.809948	-4.416636	-4.090792
16	6	0	-0.755909	-0.710935	-1.982275
17	6	0	-3.619079	-4.576606	-3.025164
18	1	0	-3.587896	-5.654081	-2.838277
19	1	0	-4.467018	-4.148270	-2.455470
20	1	0	4.327823	2.449622	-3.104145
21	6	0	3.545853	2.303591	-2.366076
22	6	0	1.558276	1.939007	-0.504970
23	6	0	2.646992	3.334582	-2.097405
24	6	0	3.445565	1.086863	-1.697125
25	6	0	2.432417	0.879682	-0.756356
26	6	0	1.638192	3.173797	-1.149417
27	1	0	2.738121	4.271482	-2.637286
28	1	0	4.141082	0.285121	-1.925405
29	6	0	0.650535	4.256375	-0.727246
30	8	0	0.572331	1.715533	0.426126
31	6	0	1.167440	4.879988	0.589948
32	1	0	2.145700	5.344986	0.427905
33	1	0	1.269926	4.117344	1.368861
34	1	0	0.466716	5.643430	0.944333
35	6	0	0.511192	5.354781	-1.780234
36	1	0	0.138645	4.949813	-2.726253
37	1	0	1.473658	5.843804	-1.954999
38	1	0	-0.177638	6.129606	-1.432299
39	6	0	-0.680822	3.574561	-0.427264
40	6	0	-3.014954	2.246064	0.419585
41	6	0	-1.939601	4.139373	-0.634919
42	6	0	-0.639598	2.327137	0.190251
43	6	0	-1.774409	1.637024	0.619753
44	6	0	-3.094181	3.485411	-0.210714
45	1	0	-2.025599	5.102738	-1.126904
46	1	0	-4.063426	3.946441	-0.373047
47	1	0	-3.920405	1.739877	0.742180
48	15	0	2.046192	-0.749509	0.002658
49	15	0	-1.498392	-0.050294	1.284177
50	6	0	-3.216642	-0.596168	1.626240
51	6	0	-5.841587	-1.509051	1.951517
52	6	0	-3.880728	-1.241844	0.575707
53	6	0	-3.878799	-0.415112	2.843133
54	6	0	-5.185314	-0.873552	3.003938
55	6	0	-5.188466	-1.690932	0.733443
56	1	0	-3.357735	-1.393943	-0.366943
57	1	0	-3.371157	0.080630	3.666262
58	1	0	-5.691305	-0.733713	3.954413
59	1	0	-5.691474	-2.191174	-0.089155
60	1	0	-6.858107	-1.867164	2.082369
61	6	0	-0.814383	0.280039	2.953411
62	6	0	0.271764	0.629847	5.505558
63	6	0	-0.907086	1.518189	3.595257
64	6	0	-0.160327	-0.778310	3.594651
65	6	0	0.369180	-0.606601	4.870206
66	6	0	-0.361146	1.692881	4.865474
67	1	0	-1.407850	2.346389	3.100439
68	1	0	-0.055515	-1.731922	3.080116
69	1	0	0.876853	-1.432291	5.358750
70	1	0	-0.435002	2.659010	5.355917
71	1	0	0.697083	0.766668	6.495420

72	6	0	3.225113	-1.855011	-0.864295
73	6	0	4.909850	-3.513181	-2.356961
74	6	0	4.549946	-2.056448	-0.464232
75	6	0	2.752142	-2.489807	-2.018659
76	6	0	3.593007	-3.311942	-2.764640
77	6	0	5.386864	-2.885902	-1.207280
78	1	0	4.925930	-1.566384	0.429942
79	1	0	1.722388	-2.325121	-2.333140
80	1	0	3.217590	-3.798249	-3.659747
81	1	0	6.413388	-3.040511	-0.889153
82	1	0	5.564183	-4.159082	-2.934376
83	6	0	2.730211	-0.645110	1.699848
84	6	0	3.692627	-0.605074	4.327833
85	6	0	2.991562	0.569429	2.336661
86	6	0	2.928199	-1.841195	2.402551
87	6	0	3.420585	-1.821689	3.702629
88	6	0	3.465825	0.587159	3.647100
89	1	0	2.831075	1.506407	1.811277
90	1	0	2.708502	-2.791992	1.921505
91	1	0	3.587163	-2.756393	4.229877
92	1	0	3.661031	1.538123	4.133378
93	1	0	4.070299	-0.588101	5.345787
94	6	0	-1.005766	0.515699	-2.728492
95	6	0	-1.491334	2.930737	-4.092660
96	6	0	0.036143	1.200075	-3.372283
97	6	0	-2.293669	1.075752	-2.769727
98	6	0	-2.531139	2.271480	-3.437869
99	6	0	-0.208498	2.387065	-4.056084
100	1	0	1.046604	0.800733	-3.317305
101	1	0	-3.104682	0.573257	-2.247388
102	1	0	-3.532288	2.693785	-3.441597
103	1	0	0.615084	2.897456	-4.548984
104	1	0	-1.677688	3.863634	-4.616969

Zero-point correction= 0.854240
(Hartree/Particle)
Thermal correction to Energy= 0.904204
Thermal correction to Enthalpy= 0.905149
Thermal correction to Gibbs Free Energy= 0.769915
Sum of electronic and zero-point Energies= -2989.920054
Sum of electronic and thermal Energies= -2989.870090
Sum of electronic and thermal Enthalpies= -2989.869145
Sum of electronic and thermal Free Energies= -2990.004379

IVb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.913723	-1.886142	0.718845

2	6	0	-4.907527	-1.887251	0.312282
3	6	0	-2.364671	-1.895274	-0.715060
4	6	0	-4.711439	-2.121956	-1.047656
5	6	0	-3.825445	-1.638062	1.151605
6	6	0	-2.521706	-1.622749	0.642871
7	6	0	-3.426743	-2.133679	-1.587524
8	1	0	-5.570395	-2.291598	-1.688817
9	1	0	-3.997953	-1.425743	2.201848
10	6	0	-3.082690	-2.397540	-3.049513
11	8	0	-1.077098	-1.884135	-1.200061
12	6	0	-2.588690	-3.856632	-3.177359
13	1	0	-3.386065	-4.549456	-2.888850
14	1	0	-1.723259	-4.035353	-2.530747
15	1	0	-2.297082	-4.063950	-4.212228
16	6	0	-4.285245	-2.190597	-3.968123
17	1	0	-4.671569	-1.168255	-3.898789
18	1	0	-5.088092	-2.886994	-3.710219
19	1	0	-4.012107	-2.393030	-5.007388
20	6	0	-1.920209	-1.474226	-3.403766
21	6	0	0.418303	0.009579	-3.904652
22	6	0	-1.729625	-0.841170	-4.631685
23	6	0	-0.926904	-1.304985	-2.440448
24	6	0	0.248577	-0.586936	-2.652305
25	6	0	-0.572160	-0.104974	-4.877408
26	1	0	-2.481200	-0.928777	-5.409495
27	1	0	-0.435171	0.374601	-5.840941
28	1	0	1.320887	0.573789	-4.115489
29	15	0	-1.043930	-1.062948	1.591230
30	15	0	1.420870	-0.455011	-1.241277
31	6	0	2.842013	0.398320	-2.033919
32	6	0	5.005231	1.810629	-3.119262
33	6	0	2.778681	1.789374	-2.188475
34	6	0	3.995606	-0.277652	-2.440642
35	6	0	5.072292	0.426825	-2.976201
36	6	0	3.850920	2.490615	-2.733041
37	1	0	1.901380	2.335854	-1.862723
38	1	0	4.067202	-1.354583	-2.322748
39	1	0	5.967054	-0.109847	-3.276707
40	1	0	3.785533	3.570001	-2.832318
41	1	0	5.848899	2.357200	-3.529920
42	6	0	2.042586	-2.168879	-1.039451
43	6	0	3.150863	-4.703092	-0.634674
44	6	0	1.736700	-3.217329	-1.909692
45	6	0	2.899783	-2.400415	0.043900
46	6	0	3.459586	-3.659360	0.235650
47	6	0	2.284328	-4.482117	-1.701665
48	1	0	1.080135	-3.050205	-2.759432
49	1	0	3.141148	-1.592557	0.732583
50	1	0	4.127553	-3.823025	1.076115
51	1	0	2.040210	-5.292195	-2.382553
52	1	0	3.581653	-5.687870	-0.478980
53	6	0	-1.828441	-0.601120	3.182127
54	6	0	-3.134286	0.190123	5.520928
55	6	0	-2.175921	-1.549052	4.149516
56	6	0	-2.138535	0.746030	3.391544
57	6	0	-2.796040	1.136728	4.556376
58	6	0	-2.822666	-1.153108	5.317793

59	1	0	-1.938469	-2.597685	3.989088
60	1	0	-1.863392	1.485195	2.641236
61	1	0	-3.032234	2.184944	4.714821
62	1	0	-3.082142	-1.893084	6.068840
63	1	0	-3.636657	0.498403	6.432882
64	6	0	-0.132796	-2.600284	2.007840
65	6	0	1.447817	-4.814095	2.652769
66	6	0	-0.272718	-3.793719	1.296943
67	6	0	0.818855	-2.517769	3.033104
68	6	0	1.599447	-3.621803	3.358365
69	6	0	0.518173	-4.894868	1.619864
70	1	0	-0.997471	-3.870613	0.491426
71	1	0	0.937141	-1.585386	3.580449
72	1	0	2.329457	-3.547451	4.158938
73	1	0	0.408345	-5.817612	1.058102
74	1	0	2.060839	-5.675438	2.900985
75	6	0	-3.844538	2.802021	-1.108519
76	8	0	-2.545606	3.263442	-1.536520
77	5	0	-1.703547	3.144220	-0.456487
78	8	0	-2.388487	2.918109	0.717050
79	6	0	-3.796297	3.070892	0.429212
80	6	0	-4.590071	2.083869	1.268961
81	1	0	-4.519037	2.352915	2.327315
82	1	0	-4.210633	1.065721	1.150931
83	1	0	-5.646964	2.102043	0.979693
84	6	0	-4.169784	4.506666	0.791875
85	1	0	-3.617278	5.221640	0.173835
86	1	0	-3.909688	4.684624	1.838982
87	1	0	-5.241494	4.686145	0.663505
88	6	0	-3.911114	1.311316	-1.438106
89	1	0	-3.153581	0.753907	-0.874506
90	1	0	-3.707122	1.172897	-2.504973
91	1	0	-4.891736	0.883516	-1.206712
92	6	0	-4.920120	3.568726	-1.859237
93	1	0	-4.788322	4.647490	-1.752670
94	1	0	-5.914131	3.295483	-1.488903
95	1	0	-4.871206	3.320493	-2.923285
96	6	0	-0.142883	3.129570	-0.567686
97	1	0	0.198092	3.692221	-1.446296
98	1	0	0.079839	2.070848	-0.786172
99	6	0	0.633238	3.553087	0.691428
100	1	0	0.023034	3.303613	1.568521
101	6	0	2.005718	2.897263	0.861473
102	6	0	3.046808	3.996975	0.758664
103	1	0	3.933972	3.713618	0.181891
104	1	0	3.390310	4.319662	1.764880
105	7	0	2.322716	5.074724	0.083521
106	6	0	0.989384	5.046361	0.679222
107	1	0	0.293739	5.660820	0.094739
108	1	0	1.013044	5.446244	1.712704
109	6	0	2.973583	6.359760	0.202722
110	1	0	3.968978	6.315813	-0.251075
111	1	0	3.089686	6.675011	1.257671
112	1	0	2.390946	7.124325	-0.321361
113	6	0	2.167834	1.594139	1.108509
114	28	0	0.689768	0.367583	0.935784
115	1	0	0.556819	0.877570	2.332201

116	1	0	2.655496	0.130587	3.265170
117	6	0	3.529689	0.167665	2.621222
118	6	0	5.732799	0.240643	0.941496
119	6	0	3.455862	0.946460	1.450231
120	6	0	4.672357	-0.555560	2.945593
121	6	0	5.779519	-0.535651	2.096729
122	6	0	4.593329	0.979811	0.627284
123	1	0	4.693622	-1.148373	3.856261
124	1	0	6.666632	-1.114377	2.335988
125	1	0	4.576693	1.567433	-0.285402
126	1	0	6.586793	0.269343	0.269861

Zero-point correction= 1.050986
(Hartree/Particle)
Thermal correction to Energy= 1.111310
Thermal correction to Enthalpy= 1.112255
Thermal correction to Gibbs Free Energy= 0.957667
Sum of electronic and zero-point Energies= -3401.485172
Sum of electronic and thermal Energies= -3401.424847
Sum of electronic and thermal Enthalpies= -3401.423903
Sum of electronic and thermal Free Energies= -3401.578491

$TS_{IIIb\text{-}IVb}$

imaginary frequencies = -98.6048 cm^{-1}

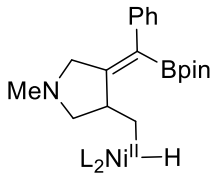
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.912765	-0.383779	0.643904
2	1	0	0.883182	-3.107750	-4.846116
3	6	0	1.151592	-2.420304	-4.050412
4	6	0	1.834525	-0.687423	-2.030371
5	6	0	2.447122	-2.428437	-3.537412
6	6	0	0.197156	-1.539355	-3.547835
7	6	0	0.525427	-0.659867	-2.515001
8	6	0	2.817145	-1.546998	-2.521266
9	1	0	3.174771	-3.127467	-3.936847
10	1	0	-0.813518	-1.551017	-3.942925
11	6	0	4.218780	-1.413271	-1.935820
12	8	0	2.136668	0.192679	-1.015615
13	6	0	4.891404	-0.180265	-2.583179
14	1	0	4.977754	-0.323376	-3.665415
15	1	0	4.308480	0.727602	-2.396090
16	1	0	5.892674	-0.038425	-2.163305
17	6	0	5.080808	-2.646052	-2.203965
18	1	0	4.645427	-3.550077	-1.765291
19	1	0	5.200866	-2.801355	-3.279989
20	1	0	6.083219	-2.505716	-1.790293
21	6	0	4.058358	-1.126757	-0.446006
22	6	0	3.719981	-0.281801	2.215174
23	6	0	4.904809	-1.591929	0.561150
24	6	0	3.031041	-0.264619	-0.067763
25	6	0	2.838836	0.187953	1.239388
26	6	0	4.733402	-1.177303	1.879535
27	1	0	5.709932	-2.277684	0.317896
28	1	0	5.403723	-1.544553	2.649849

29	1	0	3.603414	0.043766	3.244347
30	15	0	-0.691259	0.410656	-1.645922
31	15	0	1.391488	1.290113	1.538162
32	6	0	1.579280	1.623518	3.336168
33	6	0	1.760371	1.965908	6.108422
34	6	0	1.045848	0.664652	4.207913
35	6	0	2.198906	2.757790	3.867844
36	6	0	2.283479	2.928641	5.248534
37	6	0	1.144439	0.829827	5.586180
38	1	0	0.558369	-0.218487	3.799199
39	1	0	2.613460	3.510749	3.203561
40	1	0	2.761318	3.816083	5.652523
41	1	0	0.732120	0.077664	6.251598
42	1	0	1.828624	2.102224	7.183405
43	6	0	1.973996	2.860710	0.780469
44	6	0	2.715851	5.348918	-0.265922
45	6	0	3.315725	3.137014	0.496290
46	6	0	1.007173	3.836698	0.516652
47	6	0	1.377417	5.078694	0.008987
48	6	0	3.682388	4.373294	-0.030402
49	1	0	4.077738	2.387474	0.693182
50	1	0	-0.043277	3.617925	0.694249
51	1	0	0.615589	5.826807	-0.187748
52	1	0	4.726440	4.577757	-0.248511
53	1	0	3.005339	6.314334	-0.670409
54	6	0	-2.258580	-0.002864	-2.502366
55	6	0	-4.714341	-0.722067	-3.628475
56	6	0	-2.934793	-1.146062	-2.054284
57	6	0	-2.809023	0.759283	-3.535488
58	6	0	-4.036979	0.403660	-4.090345
59	6	0	-4.154967	-1.504808	-2.619034
60	1	0	-2.504217	-1.752429	-1.260038
61	1	0	-2.289984	1.640635	-3.899611
62	1	0	-4.463672	1.009487	-4.883892
63	1	0	-4.675303	-2.387205	-2.258877
64	1	0	-5.674679	-0.992672	-4.057149
65	6	0	-0.287419	2.105518	-2.224254
66	6	0	0.218195	4.729680	-3.061928
67	6	0	0.918491	2.426408	-2.853665
68	6	0	-1.232921	3.116129	-2.007023
69	6	0	-0.984601	4.416704	-2.432553
70	6	0	1.169725	3.733892	-3.264075
71	1	0	1.664015	1.660393	-3.039628
72	1	0	-2.179957	2.883291	-1.531489
73	1	0	-1.737240	5.181825	-2.264383
74	1	0	2.112383	3.970045	-3.748150
75	1	0	0.416658	5.746539	-3.388029
76	7	0	-5.164123	-1.986631	2.399505
77	6	0	-4.976372	-0.652762	1.812706
78	6	0	-3.525110	-0.659328	1.378855
79	6	0	-2.893847	-1.948609	1.833536
80	6	0	-3.863055	-2.383074	2.938979
81	1	0	-5.144528	0.149098	2.559175
82	1	0	-5.692612	-0.492084	0.997470
83	1	0	-3.626195	-1.836531	3.875563
84	1	0	-3.851471	-3.457338	3.158013
85	6	0	-6.237762	-2.038083	3.364521

86	1	0	-7.181903	-1.754504	2.887538
87	1	0	-6.068387	-1.357277	4.220982
88	1	0	-6.342927	-3.056562	3.752258
89	6	0	-2.723515	0.287700	0.881794
90	6	0	-3.199292	1.632850	0.520201
91	6	0	-4.060941	4.229360	-0.164618
92	6	0	-4.218260	1.829663	-0.426754
93	6	0	-2.621430	2.768213	1.111980
94	6	0	-3.049080	4.050637	0.780372
95	6	0	-4.642517	3.113211	-0.765700
96	1	0	-4.657560	0.960417	-0.911617
97	1	0	-1.832929	2.622732	1.848255
98	1	0	-2.589432	4.913223	1.255888
99	1	0	-5.424560	3.241936	-1.508785
100	1	0	-4.391827	5.228996	-0.430217
101	1	0	-2.943353	-2.695686	1.025047
102	6	0	-1.439313	-1.642632	2.173734
103	1	0	-0.891754	-2.525096	2.523547
104	1	0	-1.408932	-0.912488	2.993017
105	1	0	0.571518	-1.166007	0.417920
106	5	0	0.241347	-2.337657	0.612277
107	8	0	1.099111	-3.109784	1.363289
108	6	0	1.157231	-4.406949	0.733407
109	6	0	-0.171222	-4.454234	-0.099339
110	8	0	-0.429252	-3.055393	-0.353030
111	6	0	1.269313	-5.474097	1.810548
112	1	0	2.222140	-5.361002	2.335295
113	1	0	1.238661	-6.474672	1.365691
114	1	0	0.463025	-5.387796	2.541882
115	6	0	2.406209	-4.403076	-0.145082
116	1	0	3.271796	-4.162802	0.479821
117	1	0	2.323259	-3.633837	-0.920397
118	1	0	2.569460	-5.373968	-0.623947
119	6	0	-1.353335	-5.016024	0.687346
120	1	0	-1.464761	-4.519683	1.656211
121	1	0	-1.238535	-6.091271	0.856058
122	1	0	-2.270247	-4.850517	0.113929
123	6	0	-0.052897	-5.161025	-1.441338
124	1	0	0.681273	-4.668557	-2.083384
125	1	0	-1.021163	-5.135989	-1.950179
126	1	0	0.235100	-6.208870	-1.302711

Zero-point correction=	1.052018
(Hartree/Particle)	
Thermal correction to Energy=	1.111868
Thermal correction to Enthalpy=	1.112812
Thermal correction to Gibbs Free Energy=	0.957935
Sum of electronic and zero-point Energies=	-3401.450747
Sum of electronic and thermal Energies=	-3401.390898
Sum of electronic and thermal Enthalpies=	-3401.389954
Sum of electronic and thermal Free Energies=	-3401.544831

Vb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-7.164474	2.345437	-1.853751
2	6	0	-6.409136	1.644597	-1.513677
3	6	0	-4.497897	-0.126167	-0.665109
4	6	0	-6.654833	0.274839	-1.587584
5	6	0	-5.199588	2.123363	-1.018007
6	6	0	-4.208743	1.235169	-0.586017
7	6	0	-5.697851	-0.641243	-1.155399
8	1	0	-7.600582	-0.076938	-1.986415
9	1	0	-5.017745	3.192281	-0.986261
10	6	0	-5.869611	-2.157087	-1.131365
11	8	0	-3.515888	-0.990253	-0.234704
12	6	0	-6.205391	-2.583070	0.316408
13	1	0	-7.147059	-2.123332	0.634021
14	1	0	-5.416077	-2.274688	1.009656
15	1	0	-6.307472	-3.671910	0.371870
16	6	0	-6.985555	-2.626465	-2.063052
17	1	0	-6.788033	-2.345092	-3.102290
18	1	0	-7.943245	-2.195118	-1.758528
19	1	0	-7.095953	-3.713106	-2.008525
20	6	0	-4.517901	-2.762225	-1.497603
21	6	0	-1.928546	-3.792700	-1.896561
22	6	0	-4.320855	-3.918660	-2.251120
23	6	0	-3.383568	-2.139314	-0.980848
24	6	0	-2.086020	-2.613970	-1.163954
25	6	0	-3.039139	-4.430908	-2.444188
26	1	0	-5.170874	-4.433391	-2.686817
27	1	0	-2.905006	-5.339749	-3.021696
28	1	0	-0.936860	-4.206670	-2.047159
29	15	0	-2.508316	1.725855	-0.063484
30	15	0	-0.732807	-1.615732	-0.417947
31	6	0	0.738780	-2.639459	-0.808929
32	6	0	3.060738	-4.044550	-1.499146
33	6	0	1.201286	-2.645712	-2.132102
34	6	0	1.451919	-3.344027	0.162246
35	6	0	2.611354	-4.039134	-0.182700
36	6	0	2.349245	-3.349416	-2.477344
37	1	0	0.663025	-2.086405	-2.895283
38	1	0	1.112356	-3.346326	1.194169
39	1	0	3.161295	-4.576917	0.583799

40	1	0	2.697422	-3.343502	-3.505347
41	1	0	3.964686	-4.583908	-1.764681
42	6	0	-0.989663	-1.919414	1.373536
43	6	0	-1.232926	-2.314721	4.130094
44	6	0	-1.694508	-3.020943	1.867745
45	6	0	-0.415342	-1.013271	2.270915
46	6	0	-0.528236	-1.216567	3.644179
47	6	0	-1.819949	-3.213301	3.241078
48	1	0	-2.142503	-3.732529	1.179085
49	1	0	0.113802	-0.141355	1.888237
50	1	0	-0.083673	-0.504074	4.332643
51	1	0	-2.371841	-4.069700	3.616676
52	1	0	-1.331016	-2.467465	5.200723
53	6	0	-2.588010	3.537420	-0.330425
54	6	0	-2.755866	6.270166	-0.888880
55	6	0	-3.255099	4.396364	0.548325
56	6	0	-2.001427	4.058252	-1.486819
57	6	0	-2.091201	5.418909	-1.768998
58	6	0	-3.335227	5.758852	0.270879
59	1	0	-3.709546	3.998447	1.452289
60	1	0	-1.455160	3.394037	-2.152226
61	1	0	-1.632036	5.815755	-2.669049
62	1	0	-3.848794	6.421230	0.961019
63	1	0	-2.817010	7.332791	-1.102949
64	6	0	-2.548267	1.587426	1.768615
65	6	0	-2.426949	1.383805	4.556262
66	6	0	-3.493195	0.828089	2.460479
67	6	0	-1.526488	2.230393	2.483240
68	6	0	-1.473840	2.136125	3.869851
69	6	0	-3.428126	0.724835	3.849378
70	1	0	-4.289933	0.321712	1.923455
71	1	0	-0.775444	2.805344	1.946069
72	1	0	-0.684949	2.647741	4.413552
73	1	0	-4.167234	0.130614	4.378060
74	1	0	-2.383502	1.306252	5.638650
75	6	0	3.854454	1.253080	-1.505771
76	6	0	2.445833	1.719256	-1.148414
77	6	0	1.995065	2.453083	-2.426203
78	7	0	3.216153	2.711308	-3.183799
79	6	0	4.030707	1.519714	-2.982237
80	1	0	2.483595	2.406450	-0.299281
81	1	0	1.312210	1.791494	-3.000124
82	1	0	1.454895	3.383203	-2.219585
83	1	0	5.064046	1.680770	-3.299583
84	1	0	3.633180	0.653667	-3.558779
85	6	0	2.972333	3.008628	-4.575815
86	1	0	2.449104	2.181185	-5.094597
87	1	0	3.919475	3.192886	-5.093011
88	1	0	2.354848	3.908633	-4.659725
89	6	0	4.734845	0.656928	-0.681166
90	6	0	1.522828	0.539652	-0.824646
91	1	0	1.877368	0.034736	0.088617
92	1	0	1.628527	-0.193276	-1.639134
93	28	0	-0.403964	0.791424	-0.621013
94	1	0	-0.012589	2.227528	-0.450413
95	5	0	4.423563	0.453686	0.830761
96	8	0	4.982113	-0.555516	1.585246

97	8	0	3.620530	1.278886	1.586319
98	6	0	4.310461	-0.552694	2.860957
99	6	0	3.817209	0.924298	2.967613
100	6	0	3.157876	-1.549942	2.757449
101	1	0	2.612630	-1.643012	3.702491
102	1	0	3.562603	-2.529421	2.485093
103	1	0	2.452106	-1.247496	1.975921
104	6	0	5.290835	-0.979131	3.941375
105	1	0	4.829144	-0.897808	4.931499
106	1	0	6.194054	-0.366276	3.922299
107	1	0	5.580384	-2.021790	3.782363
108	6	0	2.504223	1.109770	3.711219
109	1	0	2.582676	0.734801	4.738069
110	1	0	2.250245	2.173283	3.748326
111	6	0	4.884177	1.864994	3.525441
112	1	0	5.042863	1.701316	4.595820
113	1	0	4.556591	2.897058	3.373818
114	1	0	5.836653	1.727307	3.004082
115	1	0	1.694304	0.584532	3.201252
116	1	0	7.735984	-2.800574	-1.539574
117	6	0	7.540511	-1.732760	-1.581517
118	6	0	7.030488	0.996248	-1.674303
119	6	0	6.321903	-1.235430	-1.127659
120	6	0	8.508537	-0.867230	-2.087548
121	6	0	8.249787	0.500846	-2.129949
122	6	0	6.043293	0.136008	-1.178436
123	1	0	5.569222	-1.908665	-0.726848
124	1	0	9.458915	-1.255255	-2.441412
125	1	0	9.000652	1.186039	-2.512664
126	1	0	6.834260	2.065392	-1.692951

Zero-point correction= 1.050147
(Hartree/Particle)
Thermal correction to Energy= 1.111073
Thermal correction to Enthalpy= 1.112017
Thermal correction to Gibbs Free Energy= 0.951378
Sum of electronic and zero-point Energies= -3401.463916
Sum of electronic and thermal Energies= -3401.402990
Sum of electronic and thermal Enthalpies= -3401.402046
Sum of electronic and thermal Free Energies= -3401.562685

$TS_{IIIb\text{-}Vb}$

Imaginary frequencies = -158.8413 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.507276	0.555956	0.274984
2	1	0	-1.446799	2.743394	0.789078
3	6	0	-1.077971	1.994479	1.496219
4	1	0	-0.332587	2.460168	2.151098
5	6	0	-2.196144	1.376771	2.293125
6	6	0	-3.264282	2.236624	2.972066
7	7	0	-4.269151	1.233436	3.319633
8	6	0	-4.358349	0.305409	2.184153
9	6	0	-3.035967	0.469016	1.445610

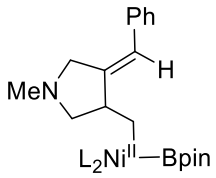
10	1	0	-1.768291	0.744329	3.092809
11	1	0	-3.650020	2.987139	2.252837
12	1	0	-2.919647	2.762795	3.869321
13	1	0	-5.179824	0.575473	1.492199
14	1	0	-4.561248	-0.714857	2.531155
15	1	0	-6.228313	0.982056	3.999682
16	6	0	-2.687468	-0.043901	0.241082
17	6	0	-5.545356	1.786883	3.708461
18	1	0	-5.415140	2.452196	4.568332
19	1	0	-6.023118	2.363423	2.893242
20	1	0	-0.794350	0.278937	-1.594885
21	5	0	-1.917168	0.805292	-1.511990
22	8	0	-2.823245	0.403556	-2.520952
23	6	0	-3.204667	1.574870	-3.252906
24	6	0	-3.030851	2.704183	-2.193043
25	8	0	-1.911668	2.226457	-1.449709
26	6	0	-4.618763	1.417505	-3.795063
27	1	0	-4.661359	0.547822	-4.457900
28	1	0	-4.901848	2.304141	-4.373319
29	1	0	-5.355805	1.280260	-3.001454
30	6	0	-2.222192	1.722244	-4.418188
31	1	0	-2.243828	0.804941	-5.013458
32	1	0	-1.203491	1.864524	-4.043545
33	1	0	-2.482075	2.565343	-5.066271
34	6	0	-4.226782	2.829138	-1.246313
35	1	0	-4.511974	1.855395	-0.836639
36	1	0	-5.092686	3.279231	-1.743063
37	1	0	-3.935730	3.467743	-0.405780
38	6	0	-2.684893	4.071611	-2.767515
39	1	0	-1.736703	4.044054	-3.310684
40	1	0	-2.593798	4.795702	-1.950941
41	1	0	-3.470343	4.421542	-3.446798
42	1	0	3.137718	-5.237503	-2.691184
43	6	0	3.110217	-4.267785	-2.204936
44	6	0	3.042821	-1.822841	-0.966225
45	6	0	4.182057	-3.389546	-2.352699
46	6	0	1.993255	-3.902124	-1.460438
47	6	0	1.932423	-2.652164	-0.832143
48	6	0	4.166320	-2.144306	-1.730303
49	1	0	5.031351	-3.681241	-2.961632
50	1	0	1.151233	-4.582117	-1.390269
51	6	0	5.282634	-1.108868	-1.800075
52	8	0	2.989119	-0.605379	-0.325875
53	6	0	6.094863	-1.171489	-0.485862
54	1	0	6.556996	-2.158274	-0.378497
55	1	0	5.454046	-0.990980	0.383179
56	1	0	6.883710	-0.411859	-0.498162
57	6	0	6.221690	-1.349338	-2.980546
58	1	0	5.687236	-1.313063	-3.935192
59	1	0	6.708108	-2.324381	-2.887946
60	1	0	7.016569	-0.598116	-2.994807
61	6	0	4.606013	0.256151	-1.867845
62	6	0	3.329268	2.752218	-1.640583
63	6	0	5.045054	1.348699	-2.613803
64	6	0	3.491864	0.446974	-1.052700
65	6	0	2.847206	1.671095	-0.897299
66	6	0	4.406233	2.582563	-2.507246

67	1	0	5.896612	1.245143	-3.278305
68	1	0	4.761181	3.425253	-3.091258
69	1	0	2.864992	3.727711	-1.543508
70	15	0	0.438704	-1.987805	0.035141
71	15	0	1.500033	1.762883	0.356972
72	6	0	1.283748	3.583892	0.416800
73	6	0	0.998079	6.360093	0.301606
74	6	0	0.435535	4.164370	-0.534048
75	6	0	1.976273	4.397797	1.314735
76	6	0	1.827243	5.782882	1.259308
77	6	0	0.303237	5.548866	-0.594168
78	1	0	-0.141416	3.530236	-1.204418
79	1	0	2.630460	3.957345	2.061135
80	1	0	2.364344	6.409422	1.964737
81	1	0	-0.352578	5.993163	-1.337201
82	1	0	0.888144	7.439293	0.256802
83	6	0	2.420362	1.322145	1.883929
84	6	0	3.773623	0.525297	4.198082
85	6	0	3.791802	1.569619	2.021418
86	6	0	1.736921	0.671554	2.914583
87	6	0	2.411133	0.274055	4.067201
88	6	0	4.462859	1.175896	3.175156
89	1	0	4.338615	2.062536	1.221120
90	1	0	0.675635	0.464163	2.811251
91	1	0	1.869034	-0.243614	4.852107
92	1	0	5.526293	1.371682	3.272871
93	1	0	4.302094	0.211930	5.093285
94	6	0	-0.778352	-3.228986	-0.543926
95	6	0	-2.529676	-5.099203	-1.651491
96	6	0	-1.482077	-2.928140	-1.714525
97	6	0	-0.969367	-4.466018	0.078405
98	6	0	-1.842564	-5.398477	-0.476204
99	6	0	-2.352784	-3.862772	-2.267414
100	1	0	-1.369046	-1.951989	-2.181584
101	1	0	-0.429837	-4.702668	0.992345
102	1	0	-1.988081	-6.358507	0.010330
103	1	0	-2.909747	-3.612828	-3.164628
104	1	0	-3.218278	-5.823661	-2.076035
105	6	0	0.729264	-2.458615	1.788244
106	6	0	1.039106	-3.051476	4.507721
107	6	0	1.863828	-3.136664	2.237112
108	6	0	-0.243050	-2.065122	2.718773
109	6	0	-0.096514	-2.370099	4.067778
110	6	0	2.019545	-3.424767	3.593253
111	1	0	2.628531	-3.444806	1.529262
112	1	0	-1.113288	-1.502041	2.381797
113	1	0	-0.861563	-2.064166	4.775402
114	1	0	2.908316	-3.948851	3.931620
115	1	0	1.160940	-3.282899	5.561637
116	6	0	-3.629042	-1.167455	-0.127178
117	6	0	-5.498401	-3.269654	-0.503648
118	6	0	-4.684066	-1.055717	-1.041123
119	6	0	-3.563793	-2.361043	0.614016
120	6	0	-4.471694	-3.396559	0.430676
121	6	0	-5.600369	-2.089877	-1.231258
122	1	0	-4.792854	-0.146721	-1.611531
123	1	0	-2.779068	-2.474279	1.356784

124	1	0	-4.375335	-4.304793	1.019183
125	1	0	-6.404730	-1.959876	-1.950439
126	1	0	-6.212687	-4.074255	-0.652480

Zero-point correction= 1.051617
(Hartree/Particle)
Thermal correction to Energy= 1.111411
Thermal correction to Enthalpy= 1.112356
Thermal correction to Gibbs Free Energy= 0.956674
Sum of electronic and zero-point Energies= -3401.417866
Sum of electronic and thermal Energies= -3401.358072
Sum of electronic and thermal Enthalpies= -3401.357128
Sum of electronic and thermal Free Energies= -3401.512809

VIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.488764	0.315545	4.703989
2	6	0	2.883533	-0.351100	3.930150
3	6	0	1.800111	-0.828153	2.950581
4	6	0	2.672990	-1.226354	1.760718
5	6	0	3.968065	-0.450045	1.862389
6	7	0	3.804027	0.373793	3.057816
7	1	0	3.389699	-1.207541	4.421142
8	1	0	4.172123	0.184539	0.988407
9	1	0	4.816149	-1.159036	1.961025
10	6	0	5.052853	0.744945	3.680662
11	1	0	5.665934	1.317097	2.975991
12	1	0	4.855435	1.376097	4.552955
13	6	0	2.347060	-2.202371	0.896927
14	28	0	0.227759	-0.087279	0.697785
15	5	0	-0.076649	-0.650604	-1.257619
16	8	0	-0.956089	-0.128774	-2.191511
17	6	0	-1.042424	-1.011403	-3.321099
18	6	0	0.308047	-1.790988	-3.236373
19	8	0	0.614313	-1.720370	-1.828140
20	1	0	1.287423	-1.721437	3.329517
21	6	0	0.774579	0.266687	2.607627
22	1	0	1.385299	-2.690185	1.067685
23	1	0	1.265078	1.236786	2.718312
24	1	0	-0.036987	0.241405	3.343639
25	6	0	-1.231132	-0.168691	-4.573823
26	1	0	-2.190746	0.354749	-4.510013
27	1	0	-1.237106	-0.795700	-5.472350
28	1	0	-0.443911	0.582482	-4.668904
29	6	0	-2.265350	-1.899203	-3.095448
30	1	0	-3.141881	-1.257724	-2.955391
31	1	0	-2.146912	-2.505097	-2.190028

32	1	0	-2.445235	-2.566385	-3.944980
33	6	0	1.452463	-1.098475	-3.972120
34	1	0	1.342770	-1.179138	-5.058660
35	1	0	2.393030	-1.576795	-3.673929
36	1	0	1.506216	-0.039397	-3.699426
37	6	0	0.227563	-3.252926	-3.649140
38	1	0	-0.478507	-3.804155	-3.021610
39	1	0	1.214225	-3.713707	-3.543693
40	1	0	-0.089601	-3.343209	-4.694368
41	1	0	5.638861	-0.132984	4.013334
42	1	0	-0.453090	4.569334	-4.053392
43	6	0	-0.769718	3.953254	-3.218170
44	6	0	-1.572672	2.349443	-1.115998
45	6	0	-2.122550	3.698188	-3.014892
46	6	0	0.174966	3.429034	-2.342614
47	6	0	-0.208622	2.614979	-1.274433
48	6	0	-2.545448	2.906130	-1.949447
49	1	0	-2.852640	4.125188	-3.694087
50	1	0	1.227344	3.637575	-2.505189
51	6	0	-4.001581	2.647617	-1.589751
52	8	0	-1.963946	1.505502	-0.095513
53	6	0	-4.369534	3.547040	-0.387043
54	1	0	-4.269591	4.602018	-0.663594
55	1	0	-3.713088	3.348742	0.465982
56	1	0	-5.403936	3.358425	-0.080426
57	6	0	-4.948833	2.960717	-2.747078
58	1	0	-4.728238	2.346232	-3.626207
59	1	0	-4.871431	4.014606	-3.028259
60	1	0	-5.987185	2.789253	-2.450558
61	6	0	-4.094341	1.195484	-1.140673
62	6	0	-4.193590	-1.387905	-0.075063
63	6	0	-5.178451	0.361550	-1.403063
64	6	0	-3.048276	0.696589	-0.355949
65	6	0	-3.074828	-0.591787	0.192487
66	6	0	-5.232107	-0.924289	-0.872428
67	1	0	-5.996631	0.716569	-2.020438
68	1	0	-6.083629	-1.563636	-1.081241
69	1	0	-4.240777	-2.395634	0.324535
70	15	0	1.004387	1.887195	-0.096884
71	15	0	-1.668808	-1.218471	1.213504
72	6	0	-1.833982	-3.048152	1.050228
73	6	0	-2.062289	-5.822689	0.696411
74	6	0	-1.035360	-3.713881	0.113160
75	6	0	-2.742373	-3.793237	1.814393
76	6	0	-2.854551	-5.169587	1.638278
77	6	0	-1.154925	-5.091976	-0.065358
78	1	0	-0.319787	-3.154117	-0.484518
79	1	0	-3.364629	-3.296963	2.553418
80	1	0	-3.562594	-5.732277	2.238879
81	1	0	-0.530491	-5.592885	-0.800511
82	1	0	-2.150688	-6.896226	0.560721
83	6	0	-2.305747	-0.944770	2.918812
84	6	0	-3.060682	-0.420022	5.565929
85	6	0	-3.250307	0.042677	3.202458
86	6	0	-1.734344	-1.661383	3.978419
87	6	0	-2.114159	-1.406869	5.291219
88	6	0	-3.624093	0.304080	4.520439

89	1	0	-3.702594	0.612150	2.395199
90	1	0	-0.990757	-2.428754	3.773609
91	1	0	-1.665454	-1.973533	6.101364
92	1	0	-4.361335	1.074402	4.725114
93	1	0	-3.353541	-0.216405	6.591247
94	6	0	2.594612	1.930581	-1.013542
95	6	0	4.990540	1.904029	-2.461230
96	6	0	3.086002	0.733623	-1.542930
97	6	0	3.331260	3.110087	-1.190666
98	6	0	4.520648	3.096892	-1.911527
99	6	0	4.275024	0.725739	-2.273925
100	1	0	2.541707	-0.196420	-1.381362
101	1	0	2.973339	4.040302	-0.757371
102	1	0	5.081105	4.017336	-2.043717
103	1	0	4.639615	-0.210868	-2.686118
104	1	0	5.917049	1.894876	-3.027255
105	6	0	1.234957	3.289039	1.077888
106	6	0	1.636163	5.329870	2.955252
107	6	0	0.327543	4.345676	1.178553
108	6	0	2.343915	3.258938	1.935099
109	6	0	2.543954	4.275350	2.862533
110	6	0	0.527516	5.360056	2.115374
111	1	0	-0.537983	4.387484	0.523476
112	1	0	3.038196	2.420525	1.903490
113	1	0	3.406856	4.237096	3.520871
114	1	0	-0.185612	6.176116	2.182674
115	1	0	1.790794	6.120751	3.682856
116	6	0	3.116556	-2.788493	-0.210776
117	6	0	4.467712	-4.068294	-2.337260
118	6	0	2.614119	-3.960840	-0.798545
119	6	0	4.322207	-2.276736	-0.714603
120	6	0	4.984778	-2.908593	-1.765848
121	6	0	3.275916	-4.595954	-1.840890
122	1	0	1.681130	-4.371592	-0.420971
123	1	0	4.744072	-1.365691	-0.307278
124	1	0	5.916007	-2.489174	-2.137163
125	1	0	2.859678	-5.502845	-2.270684
126	1	0	4.988298	-4.558380	-3.154001

Zero-point correction= 1.055081
(Hartree/Particle)
Thermal correction to Energy= 1.115077
Thermal correction to Enthalpy= 1.116022
Thermal correction to Gibbs Free Energy= 0.961697
Sum of electronic and zero-point Energies= -3401.459863
Sum of electronic and thermal Energies= -3401.399867
Sum of electronic and thermal Enthalpies= -3401.398923
Sum of electronic and thermal Free Energies= -3401.553248

$TS_{IIIb\text{-}VIb}$

Imaginary frequency: -1128.8246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.277754	-4.412063	-0.138140

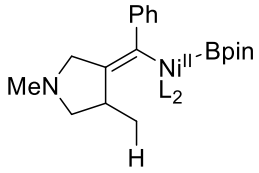
2	6	0	-3.730387	-3.475885	0.207113
3	6	0	-2.723086	-2.302283	0.245797
4	6	0	-3.472602	-1.173678	-0.406097
5	6	0	-4.918463	-1.601453	-0.501007
6	7	0	-4.773936	-3.039474	-0.724008
7	1	0	-4.158224	-3.655992	1.214146
8	1	0	-5.473329	-1.124033	-1.314793
9	1	0	-5.456740	-1.395425	0.450853
10	6	0	-6.010660	-3.772578	-0.585141
11	1	0	-6.743165	-3.412144	-1.314458
12	1	0	-5.833597	-4.836204	-0.773607
13	6	0	-2.867352	-0.088419	-0.911503
14	28	0	-0.753126	-0.615379	-0.698036
15	5	0	-0.359783	1.504709	-1.047030
16	8	0	-0.089121	2.321907	0.025681
17	6	0	-0.044011	3.682087	-0.457103
18	6	0	0.287075	3.495732	-1.978264
19	8	0	-0.193768	2.154493	-2.244366
20	1	0	-2.563617	-2.018024	1.295660
21	6	0	-1.355789	-2.472731	-0.415445
22	1	0	-1.580182	0.678034	-0.972199
23	1	0	-1.486409	-2.963204	-1.393218
24	1	0	-0.699721	-3.093330	0.208453
25	6	0	1.003573	4.438462	0.344277
26	1	0	0.708946	4.452895	1.398441
27	1	0	1.093694	5.471409	-0.009512
28	1	0	1.979839	3.950722	0.276773
29	6	0	-1.436443	4.263615	-0.209692
30	1	0	-1.659725	4.187871	0.859080
31	1	0	-2.200118	3.698604	-0.758625
32	1	0	-1.495112	5.315587	-0.505962
33	6	0	1.781492	3.504311	-2.269273
34	1	0	2.203677	4.508089	-2.154215
35	1	0	1.947475	3.167975	-3.296854
36	1	0	2.309570	2.822763	-1.599094
37	6	0	-0.443769	4.452729	-2.907712
38	1	0	-1.526549	4.336276	-2.820829
39	1	0	-0.156739	4.243933	-3.942698
40	1	0	-0.176977	5.490651	-2.680341
41	1	0	-6.449434	-3.670060	0.426650
42	1	0	5.073408	1.637653	-3.260979
43	6	0	4.496630	1.340917	-2.391169
44	6	0	3.020913	0.615303	-0.186749
45	6	0	4.798179	1.881722	-1.143648
46	6	0	3.467715	0.411982	-2.527822
47	6	0	2.710185	0.032547	-1.418528
48	6	0	4.071085	1.516525	-0.008984
49	1	0	5.616559	2.588570	-1.056078
50	1	0	3.247573	-0.013979	-3.501573
51	6	0	4.415522	1.928248	1.417686
52	8	0	2.275279	0.198355	0.885736
53	6	0	5.269013	0.798449	2.038091
54	1	0	6.199193	0.672823	1.473589
55	1	0	4.724215	-0.151914	2.027630
56	1	0	5.513478	1.040502	3.077581
57	6	0	5.209191	3.234243	1.461085
58	1	0	4.641129	4.064082	1.027391

59	1	0	6.150436	3.130263	0.914479
60	1	0	5.472075	3.489492	2.490909
61	6	0	3.113692	2.017034	2.206279
62	6	0	0.721534	1.923436	3.672468
63	6	0	2.882145	2.917674	3.245518
64	6	0	2.107368	1.093582	1.922519
65	6	0	0.907374	1.009872	2.631876
66	6	0	1.697006	2.870248	3.973779
67	1	0	3.630047	3.663168	3.494168
68	1	0	1.531558	3.577209	4.780446
69	1	0	-0.204398	1.912232	4.237905
70	15	0	1.343194	-1.196721	-1.443439
71	15	0	-0.395380	-0.146248	2.002682
72	6	0	-1.863426	0.494603	2.902261
73	6	0	-4.085683	1.699122	4.114969
74	6	0	-2.685527	1.366534	2.178165
75	6	0	-2.165759	0.238471	4.245864
76	6	0	-3.273968	0.831882	4.845424
77	6	0	-3.786639	1.970512	2.782287
78	1	0	-2.451339	1.583665	1.139273
79	1	0	-1.527394	-0.421208	4.827983
80	1	0	-3.499400	0.623114	5.886903
81	1	0	-4.407914	2.649454	2.204671
82	1	0	-4.946323	2.163617	4.586612
83	6	0	0.008679	-1.742810	2.831926
84	6	0	0.627131	-4.340328	3.717595
85	6	0	-0.992161	-2.592983	3.320513
86	6	0	1.325605	-2.220717	2.792774
87	6	0	1.630664	-3.505321	3.232179
88	6	0	-0.684697	-3.877805	3.762182
89	1	0	-2.023208	-2.255139	3.362235
90	1	0	2.122423	-1.595216	2.400708
91	1	0	2.657353	-3.855237	3.184864
92	1	0	-1.477265	-4.517391	4.139103
93	1	0	0.865691	-5.343834	4.056316
94	6	0	1.215176	-1.623974	-3.219043
95	6	0	0.946816	-2.184623	-5.941819
96	6	0	0.138413	-1.103518	-3.942501
97	6	0	2.155302	-2.432912	-3.867696
98	6	0	2.020806	-2.710749	-5.224559
99	6	0	0.006915	-1.381341	-5.301577
100	1	0	-0.600784	-0.487199	-3.434691
101	1	0	2.989671	-2.847442	-3.307128
102	1	0	2.751810	-3.340888	-5.721706
103	1	0	-0.835010	-0.977314	-5.854990
104	1	0	0.840426	-2.406988	-6.999177
105	6	0	2.168539	-2.682097	-0.732364
106	6	0	3.291186	-5.008141	0.360204
107	6	0	3.379335	-2.627148	-0.036314
108	6	0	1.537290	-3.922554	-0.893244
109	6	0	2.092851	-5.075061	-0.347454
110	6	0	3.935809	-3.783650	0.507256
111	1	0	3.908703	-1.686480	0.076639
112	1	0	0.608758	-3.986828	-1.452390
113	1	0	1.589155	-6.027564	-0.478908
114	1	0	4.878547	-3.722882	1.043263
115	1	0	3.723637	-5.908281	0.786458

116	1	0	-5.011331	1.077431	0.217990
117	6	0	-4.750031	1.549887	-0.725826
118	6	0	-4.037417	2.785847	-3.106939
119	6	0	-5.476494	2.645671	-1.183528
120	6	0	-3.656881	1.046212	-1.449411
121	6	0	-3.306981	1.693979	-2.644380
122	6	0	-5.122939	3.269872	-2.377741
123	1	0	-6.316983	3.015254	-0.602649
124	1	0	-2.448275	1.340354	-3.208398
125	1	0	-5.684772	4.127285	-2.735457
126	1	0	-3.753854	3.263844	-4.040688

Zero-point correction= 1.048313
(Hartree/Particle)
Thermal correction to Energy= 1.108686
Thermal correction to Enthalpy= 1.109631
Thermal correction to Gibbs Free Energy= 0.952294
Sum of electronic and zero-point Energies= -3401.408651
Sum of electronic and thermal Energies= -3401.348278
Sum of electronic and thermal Enthalpies= -3401.347334
Sum of electronic and thermal Free Energies= -3401.504670

VIIb



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.677061	3.837906	-2.934832
2	6	0	3.813583	3.230110	-2.032167
3	6	0	2.591032	2.376717	-1.674745
4	6	0	3.213063	1.210891	-0.906938
5	6	0	4.721783	1.326349	-1.102737
6	7	0	4.870346	2.245714	-2.226263
7	1	0	4.058985	3.914366	-1.193336
8	1	0	5.212395	0.369899	-1.308706
9	1	0	5.191841	1.743479	-0.184297
10	6	0	6.187943	2.829614	-2.320642
11	1	0	6.935730	2.042629	-2.459907
12	1	0	6.236460	3.505494	-3.180813
13	6	0	2.560827	0.272927	-0.194181
14	28	0	0.532141	0.185250	-0.512507
15	5	0	-1.143720	0.077270	-1.626516
16	8	0	-1.116762	-0.694507	-2.779994
17	6	0	-2.417474	-0.647057	-3.409367
18	6	0	-3.022275	0.669016	-2.825615
19	8	0	-2.321538	0.803378	-1.574086
20	1	0	1.910751	2.945180	-1.034292
21	6	0	1.836184	1.920957	-2.926085
22	1	0	1.028797	1.220644	-2.669939
23	1	0	2.520723	1.402914	-3.607190

24	1	0	1.390703	2.773901	-3.454428
25	6	0	-3.181308	-1.888705	-2.961784
26	1	0	-2.587610	-2.776316	-3.201136
27	1	0	-4.149254	-1.964454	-3.468420
28	1	0	-3.350622	-1.873715	-1.881615
29	6	0	-2.232291	-0.659826	-4.918867
30	1	0	-1.795419	-1.616200	-5.221141
31	1	0	-1.564828	0.139149	-5.248330
32	1	0	-3.196578	-0.548129	-5.426996
33	6	0	-4.514196	0.625084	-2.528764
34	1	0	-5.092831	0.453092	-3.443028
35	1	0	-4.822021	1.582043	-2.096253
36	1	0	-4.746813	-0.160669	-1.805255
37	6	0	-2.686187	1.901027	-3.665196
38	1	0	-1.610675	1.948769	-3.871213
39	1	0	-2.972685	2.798620	-3.108208
40	1	0	-3.223586	1.896775	-4.618642
41	1	0	6.458570	3.403964	-1.413107
42	1	0	-4.988842	3.756641	1.276735
43	6	0	-4.352461	2.877844	1.278323
44	6	0	-2.738661	0.646170	1.279876
45	6	0	-4.908235	1.618154	1.481488
46	6	0	-2.981731	3.014540	1.079689
47	6	0	-2.149905	1.893748	1.061217
48	6	0	-4.104134	0.478478	1.503373
49	1	0	-5.978324	1.528414	1.636012
50	1	0	-2.557353	3.999744	0.914377
51	6	0	-4.596667	-0.924533	1.834202
52	8	0	-1.908849	-0.452054	1.266344
53	6	0	-4.277673	-1.201446	3.321618
54	1	0	-4.817082	-0.491738	3.957826
55	1	0	-3.205395	-1.098133	3.516960
56	1	0	-4.580396	-2.219196	3.589103
57	6	0	-6.101350	-1.074458	1.611635
58	1	0	-6.374628	-0.886356	0.568044
59	1	0	-6.653554	-0.378687	2.249013
60	1	0	-6.432766	-2.079352	1.886105
61	6	0	-3.788843	-1.908197	0.994447
62	6	0	-2.102882	-3.721450	-0.317592
63	6	0	-4.290528	-3.108933	0.492427
64	6	0	-2.431441	-1.636830	0.800829
65	6	0	-1.557734	-2.526129	0.158296
66	6	0	-3.454280	-4.009853	-0.158499
67	1	0	-5.340830	-3.350070	0.615696
68	1	0	-3.856753	-4.938362	-0.549844
69	1	0	-1.476434	-4.420563	-0.857736
70	15	0	-0.352201	1.993432	0.676059
71	15	0	0.213163	-2.034329	-0.078277
72	6	0	0.866042	-3.259685	-1.265776
73	6	0	1.936709	-4.970351	-3.207776
74	6	0	1.339901	-2.748883	-2.479569
75	6	0	0.925146	-4.642259	-1.041630
76	6	0	1.460545	-5.491363	-2.005707
77	6	0	1.871929	-3.600249	-3.445521
78	1	0	1.294651	-1.678022	-2.661370
79	1	0	0.552245	-5.061177	-0.111230
80	1	0	1.505713	-6.559409	-1.817316

81	1	0	2.241033	-3.189643	-4.379996
82	1	0	2.355956	-5.634457	-3.957390
83	6	0	0.933597	-2.416751	1.579857
84	6	0	1.948516	-2.820114	4.165608
85	6	0	0.629983	-1.523101	2.617348
86	6	0	1.792258	-3.484735	1.845875
87	6	0	2.285789	-3.688495	3.133437
88	6	0	1.129508	-1.725129	3.899164
89	1	0	0.017423	-0.649903	2.423742
90	1	0	2.121606	-4.141990	1.050383
91	1	0	2.961789	-4.518469	3.317098
92	1	0	0.886859	-1.012347	4.682573
93	1	0	2.343228	-2.979451	5.164679
94	6	0	-0.227463	3.697849	0.011241
95	6	0	-0.042733	6.207902	-1.201967
96	6	0	-0.586242	3.863548	-1.331908
97	6	0	0.219857	4.797785	0.744229
98	6	0	0.314204	6.049181	0.133962
99	6	0	-0.499541	5.112250	-1.935167
100	1	0	-0.923329	2.999960	-1.899087
101	1	0	0.501586	4.680370	1.786577
102	1	0	0.668389	6.900589	0.706978
103	1	0	-0.776653	5.228221	-2.978985
104	1	0	0.038149	7.182651	-1.673013
105	6	0	0.391474	2.117325	2.353029
106	6	0	1.636153	2.250001	4.857236
107	6	0	-0.366729	2.035262	3.524741
108	6	0	1.781781	2.261479	2.445868
109	6	0	2.396590	2.340124	3.691703
110	6	0	0.255773	2.093539	4.771417
111	1	0	-1.445650	1.924303	3.470000
112	1	0	2.381743	2.279739	1.538471
113	1	0	3.474958	2.454995	3.751498
114	1	0	-0.343064	2.023954	5.674542
115	1	0	2.119805	2.300644	5.827996
116	1	0	3.440695	0.094883	2.391044
117	6	0	3.823431	-0.706356	1.764516
118	6	0	4.773038	-2.792035	0.193670
119	6	0	3.430440	-0.764309	0.418148
120	6	0	4.682594	-1.656679	2.307528
121	6	0	5.164571	-2.706777	1.527431
122	6	0	3.922973	-1.832238	-0.350812
123	1	0	4.967910	-1.583869	3.354103
124	1	0	5.831474	-3.449799	1.955335
125	1	0	3.643805	-1.890535	-1.399827
126	1	0	5.136423	-3.602999	-0.432715

Zero-point correction=	1.053290
(Hartree/Particle)	
Thermal correction to Energy=	1.114391
Thermal correction to Enthalpy=	1.115335
Thermal correction to Gibbs Free Energy=	0.957351
Sum of electronic and zero-point Energies=	-3401.456000
Sum of electronic and thermal Energies=	-3401.394899
Sum of electronic and thermal Enthalpies=	-3401.393955
Sum of electronic and thermal Free Energies=	-3401.551939

$TS_{IIIb\text{-}VIIb}$

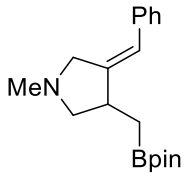
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.988934	3.309088	-3.644436
2	6	0	3.231415	3.219823	-2.578668
3	6	0	2.261380	2.295620	-1.804553
4	6	0	3.180231	1.406402	-1.000494
5	6	0	4.548748	2.039638	-1.054517
6	7	0	4.552422	2.610493	-2.404108
7	1	0	3.208763	4.238148	-2.142410
8	1	0	5.367758	1.325562	-0.923676
9	1	0	4.661677	2.837533	-0.286365
10	6	0	5.636265	3.535533	-2.640086
11	1	0	6.596807	3.027477	-2.508477
12	1	0	5.586441	3.913713	-3.666560
13	6	0	2.769372	0.197181	-0.589779
14	28	0	0.864513	-0.061855	-1.176023
15	5	0	-1.099792	-0.213655	-2.118905
16	8	0	-1.365677	-1.077297	-3.151507
17	6	0	-2.805446	-1.187927	-3.292041
18	6	0	-3.316009	0.094236	-2.552461
19	8	0	-2.242039	0.366826	-1.621652
20	1	0	1.648068	2.919483	-1.141206
21	6	0	1.343546	1.410322	-2.641256
22	1	0	0.039002	0.639977	-2.314504
23	1	0	1.926005	0.763895	-3.307333
24	1	0	0.669680	2.017757	-3.260336
25	6	0	-3.236499	-2.475487	-2.602261
26	1	0	-2.652616	-3.308925	-3.004620
27	1	0	-4.299603	-2.675465	-2.771250
28	1	0	-3.059026	-2.421627	-1.526630
29	6	0	-3.139792	-1.243961	-4.774725
30	1	0	-2.750323	-2.173191	-5.200160
31	1	0	-2.697540	-0.406081	-5.317586
32	1	0	-4.224969	-1.228078	-4.922537
33	6	0	-4.609621	-0.081293	-1.773661
34	1	0	-5.432738	-0.331677	-2.452231
35	1	0	-4.852804	0.853896	-1.258760
36	1	0	-4.518910	-0.867345	-1.019522
37	6	0	-3.415341	1.315437	-3.465989
38	1	0	-2.474673	1.477776	-4.004775
39	1	0	-3.617429	2.198095	-2.851394
40	1	0	-4.222393	1.207763	-4.196744
41	1	0	5.606741	4.403639	-1.952483
42	1	0	-5.351468	3.360553	1.371537
43	6	0	-4.616967	2.561529	1.365633
44	6	0	-2.759783	0.528493	1.339020
45	6	0	-5.000134	1.264552	1.694753
46	6	0	-3.290595	2.838521	1.042930
47	6	0	-2.334744	1.821500	1.022223

48	6	0	-4.071329	0.223171	1.698870
49	1	0	-6.034204	1.067472	1.956593
50	1	0	-2.995368	3.853146	0.792125
51	6	0	-4.373591	-1.197190	2.155405
52	8	0	-1.803688	-0.461539	1.294178
53	6	0	-3.939717	-1.321703	3.634489
54	1	0	-4.518255	-0.628210	4.254015
55	1	0	-2.876790	-1.086844	3.750401
56	1	0	-4.108934	-2.342977	3.991938
57	6	0	-5.861004	-1.533049	2.043517
58	1	0	-6.213903	-1.461264	1.009232
59	1	0	-6.454028	-0.855309	2.662910
60	1	0	-6.056545	-2.542748	2.413753
61	6	0	-3.503898	-2.149476	1.341796
62	6	0	-1.682939	-3.899221	0.128928
63	6	0	-3.882078	-3.448954	1.005474
64	6	0	-2.205773	-1.741161	1.014834
65	6	0	-1.262106	-2.600210	0.431798
66	6	0	-2.980879	-4.317483	0.400067
67	1	0	-4.885259	-3.795526	1.229083
68	1	0	-3.287711	-5.324986	0.139526
69	1	0	-1.002971	-4.587549	-0.356759
70	15	0	-0.573852	2.053707	0.529687
71	15	0	0.446080	-1.982579	0.051474
72	6	0	1.164351	-3.375399	-0.898343
73	6	0	2.280593	-5.388480	-2.498751
74	6	0	1.480686	-3.127575	-2.238906
75	6	0	1.388300	-4.658047	-0.378530
76	6	0	1.950523	-5.654444	-1.170601
77	6	0	2.035149	-4.127861	-3.034797
78	1	0	1.306226	-2.139966	-2.659518
79	1	0	1.110785	-4.885947	0.646513
80	1	0	2.125326	-6.640129	-0.750951
81	1	0	2.280594	-3.915678	-4.070552
82	1	0	2.721417	-6.165979	-3.115047
83	6	0	1.251117	-1.961185	1.713588
84	6	0	2.415436	-1.695937	4.254090
85	6	0	0.899010	-0.901589	2.557960
86	6	0	2.226796	-2.864519	2.143756
87	6	0	2.793089	-2.736107	3.410334
88	6	0	1.474986	-0.767442	3.816886
89	1	0	0.180138	-0.164283	2.229326
90	1	0	2.596354	-3.640086	1.485096
91	1	0	3.558153	-3.441144	3.721521
92	1	0	1.191587	0.076549	4.440106
93	1	0	2.870321	-1.595745	5.235066
94	6	0	-0.679815	3.701562	-0.283871
95	6	0	-0.825121	6.087617	-1.744834
96	6	0	-1.149739	3.702576	-1.604262
97	6	0	-0.279455	4.908073	0.294758
98	6	0	-0.349365	6.094409	-0.436772
99	6	0	-1.230237	4.886793	-2.328050
100	1	0	-1.451631	2.760887	-2.057510
101	1	0	0.092656	4.924605	1.315453
102	1	0	-0.031193	7.026477	0.020808
103	1	0	-1.598911	4.872019	-3.349692
104	1	0	-0.875949	7.012952	-2.310334

105	6	0	0.220459	2.474163	2.137668
106	6	0	1.619031	3.073180	4.491436
107	6	0	-0.467373	2.667034	3.338918
108	6	0	1.619642	2.569066	2.130772
109	6	0	2.312493	2.878056	3.297319
110	6	0	0.230936	2.959972	4.511173
111	1	0	-1.551119	2.591665	3.362064
112	1	0	2.165564	2.373828	1.208353
113	1	0	3.395910	2.953947	3.275996
114	1	0	-0.313397	3.106678	5.439411
115	1	0	2.159479	3.306066	5.403883
116	1	0	3.909731	0.666336	1.812532
117	6	0	4.269535	-0.258408	1.367009
118	6	0	5.147680	-2.642566	0.249133
119	6	0	3.741427	-0.655923	0.128079
120	6	0	5.215534	-1.031041	2.032076
121	6	0	5.661086	-2.229712	1.477544
122	6	0	4.197288	-1.868519	-0.412781
123	1	0	5.599574	-0.700470	2.993759
124	1	0	6.399639	-2.834088	1.996309
125	1	0	3.809923	-2.193750	-1.374389
126	1	0	5.490337	-3.571518	-0.199663

Zero-point correction= 1.049429
(Hartree/Particle)
Thermal correction to Energy= 1.109604
Thermal correction to Enthalpy= 1.110548
Thermal correction to Gibbs Free Energy= 0.956248
Sum of electronic and zero-point Energies= -3401.415742
Sum of electronic and thermal Energies= -3401.355567
Sum of electronic and thermal Enthalpies= -3401.354623
Sum of electronic and thermal Free Energies= -3401.508923

2B

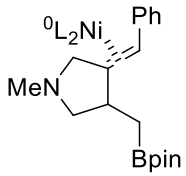


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.897019	1.582535	0.794271
2	6	0	-0.867899	2.057623	-0.637153
3	7	0	0.558392	2.267427	-0.849038
4	6	0	1.024499	2.941300	0.356776
5	6	0	0.301754	2.207640	1.505199
6	1	0	-1.439444	3.002022	-0.762840
7	1	0	-1.269854	1.323137	-1.343831
8	1	0	0.741017	4.011202	0.345722
9	1	0	2.115113	2.873216	0.428722
10	1	0	-0.039321	2.934671	2.251694
11	6	0	-1.688013	0.641992	1.317462
12	5	0	1.663157	0.051276	1.187370

13	8	0	0.991657	-1.132946	1.010743
14	6	0	1.471321	-1.703813	-0.225081
15	6	0	2.901670	-1.077392	-0.344004
16	8	0	2.757185	0.170211	0.369168
17	6	0	1.200363	1.160751	2.203466
18	1	0	0.642778	0.697476	3.025339
19	1	0	2.059959	1.677390	2.645421
20	6	0	0.876933	2.967051	-2.072764
21	1	0	0.516001	2.392527	-2.932050
22	1	0	1.962226	3.073955	-2.162182
23	6	0	-2.765270	-0.074868	0.613261
24	6	0	-4.755071	-1.529452	-0.735828
25	6	0	-3.613607	0.554815	-0.305844
26	6	0	-2.947063	-1.443529	0.860136
27	6	0	-3.927049	-2.165875	0.188100
28	6	0	-4.597177	-0.166961	-0.977093
29	1	0	-3.516000	1.623554	-0.475047
30	1	0	-2.292835	-1.939175	1.573338
31	1	0	-4.046807	-3.226895	0.385659
32	1	0	-5.248277	0.339176	-1.683549
33	1	0	-5.523987	-2.090344	-1.257869
34	6	0	0.522534	-1.224784	-1.322942
35	1	0	0.576102	-0.134632	-1.415202
36	1	0	-0.500804	-1.500056	-1.046705
37	1	0	0.763156	-1.682539	-2.287874
38	6	0	1.440548	-3.219465	-0.115117
39	1	0	1.989829	-3.569529	0.761541
40	1	0	1.874108	-3.678219	-1.010362
41	1	0	0.402692	-3.554637	-0.027857
42	6	0	3.346045	-0.775847	-1.766392
43	1	0	2.676550	-0.053530	-2.238474
44	1	0	3.365276	-1.691092	-2.367762
45	1	0	4.354918	-0.353083	-1.753522
46	6	0	3.966868	-1.887952	0.391037
47	1	0	4.889043	-1.301955	0.435819
48	1	0	4.178008	-2.831264	-0.121901
49	1	0	3.650049	-2.108545	1.415297
50	1	0	-1.483405	0.303188	2.332594
51	1	0	0.422443	3.974893	-2.111919

Zero-point correction= 0.450067
(Hartree/Particle)
Thermal correction to Energy= 0.472160
Thermal correction to Enthalpy= 0.473104
Thermal correction to Gibbs Free Energy= 0.399418
Sum of electronic and zero-point Energies= -970.154518
Sum of electronic and thermal Energies= -970.132425
Sum of electronic and thermal Enthalpies= -970.131481
Sum of electronic and thermal Free Energies= -970.205168

2B-Ni



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.814281	-4.666537	4.304596
2	6	0	-1.919534	-3.711714	3.799858
3	6	0	-2.196817	-1.302347	2.517965
4	6	0	-2.416377	-2.611851	4.496160
5	6	0	-1.549517	-3.595791	2.463420
6	6	0	-1.665068	-2.371262	1.796405
7	6	0	-2.574245	-1.382686	3.859351
8	1	0	-2.687053	-2.720877	5.541247
9	1	0	-1.150682	-4.459529	1.941798
10	6	0	-3.175439	-0.131649	4.493206
11	8	0	-2.350013	-0.113560	1.843493
12	6	0	-4.649651	-0.022586	4.041395
13	1	0	-5.215780	-0.890799	4.394757
14	1	0	-4.723563	0.021205	2.950381
15	1	0	-5.100514	0.886076	4.453650
16	6	0	-3.124360	-0.177655	6.019601
17	1	0	-2.096316	-0.260282	6.386396
18	1	0	-3.700259	-1.027855	6.395773
19	1	0	-3.576372	0.723276	6.443562
20	6	0	-2.416426	1.064474	3.926232
21	6	0	-1.135525	3.209790	2.637748
22	6	0	-2.092397	2.223768	4.629186
23	6	0	-2.067344	1.016878	2.576339
24	6	0	-1.428104	2.056382	1.903070
25	6	0	-1.461174	3.289150	3.989285
26	1	0	-2.333704	2.303695	5.684097
27	1	0	-1.219058	4.186234	4.549760
28	1	0	-0.635517	4.042037	2.151676
29	15	0	-1.054147	-2.058255	0.078134
30	15	0	-1.004361	1.789379	0.124964
31	6	0	0.124864	3.218368	-0.124030
32	6	0	2.031038	5.242821	-0.470437
33	6	0	1.451159	3.031078	0.292249
34	6	0	-0.233085	4.427799	-0.721195
35	6	0	0.719261	5.434394	-0.894920
36	6	0	2.397306	4.036345	0.127813
37	1	0	1.757403	2.078600	0.725408
38	1	0	-1.251002	4.582715	-1.068257
39	1	0	0.431877	6.368504	-1.368411
40	1	0	3.419498	3.861259	0.451087
41	1	0	2.768921	6.026407	-0.612310

42	6	0	-2.577304	2.266276	-0.694537
43	6	0	-4.935162	2.903158	-2.055622
44	6	0	-3.389831	3.315946	-0.246795
45	6	0	-2.970302	1.526195	-1.812559
46	6	0	-4.141472	1.848742	-2.495413
47	6	0	-4.561389	3.634151	-0.926651
48	1	0	-3.104406	3.882423	0.636983
49	1	0	-2.358904	0.695196	-2.154951
50	1	0	-4.422762	1.268098	-3.368639
51	1	0	-5.185225	4.450977	-0.576256
52	1	0	-5.848787	3.156103	-2.585381
53	6	0	-0.330629	-3.709085	-0.283355
54	6	0	0.943452	-6.174323	-0.673431
55	6	0	-0.983628	-4.742485	-0.960379
56	6	0	0.962266	-3.929057	0.202972
57	6	0	1.594905	-5.154462	0.018956
58	6	0	-0.343458	-5.964977	-1.162222
59	1	0	-1.994081	-4.598324	-1.330752
60	1	0	1.475957	-3.127091	0.729896
61	1	0	2.599450	-5.307144	0.402038
62	1	0	-0.857649	-6.757963	-1.696548
63	1	0	1.436944	-7.128338	-0.830611
64	6	0	-2.599097	-2.034096	-0.919893
65	6	0	-4.817849	-1.721256	-2.604217
66	6	0	-3.855567	-1.738178	-0.386779
67	6	0	-2.471650	-2.187068	-2.306446
68	6	0	-3.571207	-2.035348	-3.144014
69	6	0	-4.956488	-1.579236	-1.226796
70	1	0	-3.984814	-1.625968	0.684916
71	1	0	-1.500795	-2.439052	-2.727193
72	1	0	-3.453541	-2.161029	-4.216367
73	1	0	-5.925501	-1.340433	-0.799254
74	1	0	-5.677243	-1.592753	-3.255375
75	6	0	6.716197	0.327922	1.154526
76	8	0	6.077682	-0.039442	-0.087342
77	5	0	4.862915	0.600917	-0.129948
78	8	0	4.556575	1.217258	1.066840
79	6	0	5.498288	0.728905	2.045322
80	6	0	5.780718	1.824720	3.059679
81	1	0	4.872975	2.038607	3.631120
82	1	0	6.102390	2.746162	2.569746
83	1	0	6.560914	1.507010	3.759889
84	6	0	4.843760	-0.473821	2.723872
85	1	0	4.651040	-1.271713	1.998057
86	1	0	3.886587	-0.160283	3.150112
87	1	0	5.471057	-0.873819	3.526132
88	6	0	7.639047	1.506059	0.850002
89	1	0	7.066246	2.371403	0.501874
90	1	0	8.333093	1.213096	0.057709
91	1	0	8.217729	1.799648	1.731010
92	6	0	7.520499	-0.856785	1.665147
93	1	0	6.905314	-1.756601	1.729861
94	1	0	7.936965	-0.640995	2.654951
95	1	0	8.349585	-1.058204	0.980920
96	6	0	3.846240	0.568815	-1.315630
97	1	0	4.315750	0.400930	-2.290929
98	1	0	3.337636	1.537975	-1.350927

99	6	0	2.822650	-0.567267	-1.063328
100	1	0	2.537298	-0.551299	0.000295
101	6	0	1.566887	-0.520571	-1.967179
102	6	0	1.679078	-1.709796	-2.916434
103	1	0	1.442436	-1.454480	-3.955168
104	1	0	1.021043	-2.552097	-2.614405
105	7	0	3.084783	-2.105633	-2.824000
106	6	0	3.442814	-1.925477	-1.423662
107	1	0	4.532899	-1.939080	-1.299982
108	1	0	3.018794	-2.732871	-0.801289
109	6	0	3.325866	-3.447142	-3.305909
110	1	0	3.047760	-3.517997	-4.362506
111	1	0	2.745750	-4.205181	-2.743611
112	1	0	4.389762	-3.689238	-3.215672
113	6	0	0.993114	0.734467	-2.262258
114	28	0	-0.007297	-0.139055	-0.738967
115	1	0	1.482095	1.615688	-1.854006
116	1	0	-1.172109	3.904485	-4.827733
117	6	0	-1.042194	2.844939	-4.625436
118	6	0	-0.690946	0.144325	-4.082791
119	6	0	-1.795614	1.902885	-5.324441
120	6	0	-0.122844	2.437470	-3.666561
121	6	0	0.069221	1.077870	-3.357854
122	6	0	-1.606644	0.550275	-5.049183
123	1	0	-2.515865	2.218724	-6.072986
124	1	0	0.459687	3.180975	-3.127128
125	1	0	-2.181814	-0.199079	-5.586710
126	1	0	-0.589059	-0.911493	-3.864345

Zero-point correction=	1.055717
(Hartree/Particle)	
Thermal correction to Energy=	1.116107
Thermal correction to Enthalpy=	1.117052
Thermal correction to Gibbs Free Energy=	0.959414
Sum of electronic and zero-point Energies=	-3401.513008
Sum of electronic and thermal Energies=	-3401.452618
Sum of electronic and thermal Enthalpies=	-3401.451674
Sum of electronic and thermal Free Energies=	-3401.609312

$TS_{IVb\text{-}2B}$

Imaginary frequency: -669.7744

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.233855	0.086243	0.183126
2	1	0	-3.399957	0.476160	2.980779
3	6	0	-3.041733	0.352859	1.947906
4	1	0	-2.110816	0.930672	1.878447
5	6	0	-2.763801	-1.135956	1.677284
6	6	0	-3.893964	-2.061895	2.143576
7	7	0	-3.775579	-3.219836	1.267505
8	6	0	-3.539173	-2.664005	-0.060110
9	6	0	-2.609128	-1.495813	0.200441
10	1	0	-1.837223	-1.434549	2.195189
11	1	0	-4.871566	-1.559604	2.016332

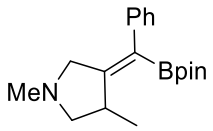
12	1	0	-3.796450	-2.360828	3.193628
13	1	0	-4.492922	-2.313730	-0.511717
14	1	0	-3.114388	-3.423808	-0.729277
15	1	0	-4.748136	-4.958772	0.649224
16	6	0	-1.700532	-0.919185	-0.612920
17	6	0	-4.912251	-4.107917	1.319452
18	1	0	-5.036349	-4.494161	2.336237
19	1	0	-5.854641	-3.609182	1.019896
20	1	0	-1.453862	0.680024	-0.486315
21	5	0	-4.077465	0.965933	0.932929
22	8	0	-5.159942	0.289958	0.418562
23	6	0	-5.660389	1.063897	-0.691077
24	6	0	-5.189309	2.508377	-0.326608
25	8	0	-4.002586	2.254431	0.453136
26	6	0	-7.167512	0.885641	-0.779364
27	1	0	-7.395875	-0.155751	-1.023659
28	1	0	-7.584410	1.522093	-1.567437
29	1	0	-7.655751	1.129718	0.166318
30	6	0	-4.984511	0.520782	-1.948274
31	1	0	-5.238920	-0.538384	-2.048452
32	1	0	-3.894028	0.600465	-1.875890
33	1	0	-5.323680	1.043629	-2.847662
34	6	0	-6.170941	3.243618	0.582780
35	1	0	-6.448650	2.624027	1.441162
36	1	0	-7.080522	3.525795	0.043984
37	1	0	-5.693362	4.153459	0.958307
38	6	0	-4.817094	3.371452	-1.522062
39	1	0	-3.974577	2.941228	-2.068062
40	1	0	-4.531572	4.372425	-1.185447
41	1	0	-5.669275	3.471668	-2.202984
42	1	0	3.400110	-4.711171	-2.488470
43	6	0	3.277221	-3.696058	-2.125640
44	6	0	2.986105	-1.133552	-1.200404
45	6	0	3.827006	-2.635623	-2.842934
46	6	0	2.552746	-3.464548	-0.959489
47	6	0	2.368230	-2.161997	-0.486810
48	6	0	3.698177	-1.325375	-2.383648
49	1	0	4.363756	-2.837513	-3.764075
50	1	0	2.098301	-4.297559	-0.433870
51	6	0	4.307292	-0.091879	-3.045328
52	8	0	2.834708	0.137128	-0.698329
53	6	0	5.604422	0.270772	-2.286634
54	1	0	6.328195	-0.546951	-2.367750
55	1	0	5.400137	0.449701	-1.225935
56	1	0	6.046160	1.177965	-2.712317
57	6	0	4.638911	-0.332109	-4.517138
58	1	0	3.746343	-0.594192	-5.094470
59	1	0	5.370495	-1.138437	-4.618767
60	1	0	5.089674	0.561918	-4.956917
61	6	0	3.319165	1.056411	-2.857449
62	6	0	1.609578	3.198809	-2.199796
63	6	0	3.071211	2.078512	-3.774621
64	6	0	2.661199	1.134361	-1.632503
65	6	0	1.817064	2.182535	-1.266133
66	6	0	2.224173	3.136706	-3.449197
67	1	0	3.545159	2.058828	-4.750599
68	1	0	2.046979	3.923243	-4.175386

69	1	0	0.957021	4.030756	-1.952307
70	15	0	1.188799	-1.689075	0.853070
71	15	0	0.999034	2.038294	0.372918
72	6	0	0.158221	3.661347	0.548347
73	6	0	-1.210082	6.078601	0.859575
74	6	0	-1.236129	3.692876	0.498671
75	6	0	0.867385	4.852286	0.752445
76	6	0	0.185360	6.055327	0.899459
77	6	0	-1.918404	4.897689	0.661788
78	1	0	-1.793433	2.776242	0.334447
79	1	0	1.953340	4.834292	0.804849
80	1	0	0.740018	6.975517	1.056500
81	1	0	-3.004329	4.894705	0.647709
82	1	0	-1.738540	7.018314	0.990249
83	6	0	2.415400	2.274872	1.528029
84	6	0	4.427460	2.696245	3.429549
85	6	0	3.704795	2.633579	1.125840
86	6	0	2.148253	2.118518	2.891755
87	6	0	3.144711	2.335522	3.837322
88	6	0	4.706380	2.839815	2.073484
89	1	0	3.931172	2.763065	0.070674
90	1	0	1.152435	1.820843	3.214280
91	1	0	2.923855	2.204778	4.892382
92	1	0	5.704313	3.119253	1.748862
93	1	0	5.207552	2.857794	4.167368
94	6	0	0.442681	-3.323169	1.246433
95	6	0	-0.779628	-5.803830	1.697141
96	6	0	-0.432158	-3.869394	0.296873
97	6	0	0.709757	-4.042783	2.414989
98	6	0	0.096564	-5.273937	2.639805
99	6	0	-1.034340	-5.103237	0.520847
100	1	0	-0.628672	-3.334276	-0.628360
101	1	0	1.402157	-3.650452	3.152291
102	1	0	0.311947	-5.820470	3.552959
103	1	0	-1.712160	-5.512273	-0.222681
104	1	0	-1.258377	-6.761856	1.875545
105	6	0	2.245544	-1.349255	2.312366
106	6	0	3.733501	-0.822492	4.622914
107	6	0	3.636497	-1.258202	2.248842
108	6	0	1.602967	-1.140334	3.540168
109	6	0	2.343052	-0.899696	4.692455
110	6	0	4.375324	-0.985322	3.399181
111	1	0	4.147695	-1.407061	1.301901
112	1	0	0.516222	-1.188516	3.595730
113	1	0	1.835053	-0.760406	5.642117
114	1	0	5.456524	-0.907702	3.336697
115	1	0	4.312391	-0.620359	5.519182
116	1	0	-3.500619	-2.029523	-2.440691
117	6	0	-2.501954	-1.890387	-2.838348
118	6	0	0.017367	-1.473594	-3.939145
119	6	0	-2.238538	-2.272167	-4.151742
120	6	0	-1.508589	-1.306143	-2.033199
121	6	0	-0.254261	-1.085676	-2.632497
122	6	0	-0.975882	-2.078199	-4.707394
123	1	0	-3.029446	-2.721258	-4.746099
124	1	0	0.521524	-0.594213	-2.050356
125	1	0	-0.773736	-2.381208	-5.730331

126	1	0	1.006602	-1.296501	-4.353983

Zero-point correction= 1.050021
(Hartree/Particle)
Thermal correction to Energy= 1.110020
Thermal correction to Enthalpy= 1.110964
Thermal correction to Gibbs Free Energy= 0.955185
Sum of electronic and zero-point Energies= -3401.479464
Sum of electronic and thermal Energies= -3401.419465
Sum of electronic and thermal Enthalpies= -3401.418521
Sum of electronic and thermal Free Energies= -3401.574299

11B



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.487116	-0.748287	0.110950
2	6	0	2.996091	-0.593617	0.097527
3	7	0	3.486817	-1.922369	-0.246302
4	6	0	2.576928	-2.831665	0.440140
5	6	0	1.197094	-2.244473	0.118224
6	1	0	3.347905	-0.296542	1.107052
7	1	0	3.347329	0.168930	-0.606609
8	1	0	2.755691	-2.828865	1.533843
9	1	0	2.705779	-3.856355	0.074490
10	1	0	0.452165	-2.498804	0.875120
11	6	0	0.585500	0.252708	0.068112
12	5	0	-0.950119	-0.019031	0.088660
13	8	0	-1.534929	-1.219502	0.424273
14	6	0	-2.938089	-1.117137	0.097740
15	6	0	-3.175539	0.424335	0.155049
16	8	0	-1.881529	0.945234	-0.215073
17	6	0	0.714602	-2.717810	-1.258776
18	1	0	1.493913	-2.539958	-2.005811
19	1	0	-0.190487	-2.184664	-1.558079
20	1	0	0.491495	-3.789929	-1.237151
21	6	0	4.877327	-2.122363	0.094964
22	1	0	5.501655	-1.413161	-0.457066
23	1	0	5.183522	-3.135886	-0.180860
24	6	0	1.032348	1.675293	-0.004109
25	6	0	1.874243	4.353865	-0.171095
26	6	0	1.908624	2.214440	0.945137
27	6	0	0.568323	2.511633	-1.027476
28	6	0	0.989991	3.834499	-1.115123
29	6	0	2.328702	3.539585	0.862709
30	1	0	2.249311	1.590177	1.766546
31	1	0	-0.130669	2.113638	-1.756808
32	1	0	0.625524	4.463600	-1.921827
33	1	0	3.008262	3.936880	1.610864
34	1	0	2.201264	5.386994	-0.237644

35	6	0	-3.742735	-1.924990	1.102642
36	1	0	-3.499898	-1.639932	2.128093
37	1	0	-3.521879	-2.989124	0.980087
38	1	0	-4.815565	-1.776688	0.939170
39	6	0	-3.110975	-1.691667	-1.307137
40	1	0	-2.547447	-1.105861	-2.041150
41	1	0	-4.163186	-1.709089	-1.606351
42	1	0	-2.728554	-2.716250	-1.319101
43	6	0	-3.467020	0.924629	1.568619
44	1	0	-2.727475	0.540969	2.278527
45	1	0	-4.464058	0.622173	1.902671
46	1	0	-3.412177	2.016402	1.574185
47	6	0	-4.219609	0.946721	-0.818221
48	1	0	-4.316167	2.030123	-0.704738
49	1	0	-5.194944	0.492443	-0.612928
50	1	0	-3.942964	0.733712	-1.852764
51	1	0	5.068668	-1.983253	1.176190

Zero-point correction= 0.449780
(Hartree/Particle)
Thermal correction to Energy= 0.472357
Thermal correction to Enthalpy= 0.473301
Thermal correction to Gibbs Free Energy= 0.399040
Sum of electronic and zero-point Energies= -970.157817
Sum of electronic and thermal Energies= -970.135239
Sum of electronic and thermal Enthalpies= -970.134295
Sum of electronic and thermal Free Energies= -970.208556

$TS_{Vb\text{-}11B}$

Imaginary frequencies = -815.3482 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-7.119045	1.940932	-2.291494
2	6	0	-6.372338	1.305365	-1.826631
3	6	0	-4.479502	-0.301871	-0.659944
4	6	0	-6.592867	-0.067122	-1.735069
5	6	0	-5.199448	1.869014	-1.332546
6	6	0	-4.218049	1.067642	-0.739701
7	6	0	-5.646590	-0.898721	-1.138786
8	1	0	-7.511281	-0.486536	-2.132273
9	1	0	-5.036313	2.937460	-1.427119
10	6	0	-5.805333	-2.401483	-0.921643
11	8	0	-3.511396	-1.089852	-0.076791
12	6	0	-6.217665	-2.634509	0.549525
13	1	0	-7.184067	-2.158536	0.746070
14	1	0	-5.476216	-2.215050	1.236392
15	1	0	-6.305575	-3.707687	0.748493
16	6	0	-6.866067	-3.008197	-1.838704
17	1	0	-6.615028	-2.866105	-2.894672
18	1	0	-7.842290	-2.554429	-1.646602
19	1	0	-6.971031	-4.079216	-1.644059
20	6	0	-4.431829	-3.029587	-1.137690
21	6	0	-1.814430	-4.047524	-1.323977
22	6	0	-4.190387	-4.270907	-1.725872

23	6	0	-3.328120	-2.322648	-0.663445
24	6	0	-2.015733	-2.787777	-0.754096
25	6	0	-2.895312	-4.779297	-1.809781
26	1	0	-5.016744	-4.853993	-2.119098
27	1	0	-2.728505	-5.752354	-2.260191
28	1	0	-0.807703	-4.446614	-1.402963
29	15	0	-2.551956	1.670435	-0.217792
30	15	0	-0.701775	-1.647857	-0.164339
31	6	0	0.844463	-2.529354	-0.611403
32	6	0	3.369661	-3.457554	-1.405689
33	6	0	1.169938	-2.640258	-1.970631
34	6	0	1.798801	-2.894569	0.340661
35	6	0	3.058778	-3.344377	-0.054771
36	6	0	2.416010	-3.115890	-2.365057
37	1	0	0.445339	-2.337039	-2.724988
38	1	0	1.566055	-2.820790	1.398773
39	1	0	3.799574	-3.598601	0.697394
40	1	0	2.650859	-3.200153	-3.422242
41	1	0	4.354695	-3.796142	-1.711667
42	6	0	-0.796656	-1.883547	1.653901
43	6	0	-0.819202	-2.152782	4.436176
44	6	0	-1.171365	-3.096528	2.241444
45	6	0	-0.439207	-0.808039	2.470822
46	6	0	-0.448123	-0.941958	3.858367
47	6	0	-1.182427	-3.229344	3.626649
48	1	0	-1.452518	-3.937413	1.612210
49	1	0	-0.157477	0.138455	2.012895
50	1	0	-0.176593	-0.094519	4.481314
51	1	0	-1.474587	-4.173552	4.076362
52	1	0	-0.831139	-2.259540	5.516661
53	6	0	-2.677864	3.455535	-0.636886
54	6	0	-2.848589	6.143403	-1.392464
55	6	0	-3.446539	4.353640	0.112568
56	6	0	-1.992024	3.918331	-1.762412
57	6	0	-2.082029	5.255760	-2.143232
58	6	0	-3.529151	5.691643	-0.262210
59	1	0	-3.979699	4.002939	0.993239
60	1	0	-1.371665	3.225769	-2.326565
61	1	0	-1.543778	5.605110	-3.019118
62	1	0	-4.123458	6.382103	0.328492
63	1	0	-2.911027	7.187813	-1.682602
64	6	0	-2.657835	1.718248	1.618996
65	6	0	-2.577256	1.757820	4.417967
66	6	0	-3.623126	1.037832	2.361713
67	6	0	-1.644723	2.417313	2.292456
68	6	0	-1.609272	2.442728	3.682045
69	6	0	-3.579051	1.055381	3.755988
70	1	0	-4.417554	0.494562	1.858247
71	1	0	-0.880252	2.938549	1.718910
72	1	0	-0.822638	2.992075	4.191533
73	1	0	-4.334514	0.519726	4.322701
74	1	0	-2.547219	1.771308	5.503368
75	6	0	3.789829	1.102626	-1.664858
76	6	0	2.452211	1.771061	-1.369252
77	6	0	2.085091	2.425363	-2.713653
78	7	0	3.338167	2.495374	-3.455977
79	6	0	4.008151	1.236456	-3.153978

80	1	0	2.573171	2.527225	-0.588971
81	1	0	1.348893	1.783503	-3.241876
82	1	0	1.638293	3.419468	-2.603087
83	1	0	5.063178	1.256668	-3.446232
84	1	0	3.523812	0.391177	-3.692288
85	6	0	3.155240	2.717823	-4.871902
86	1	0	2.552306	1.918930	-5.346364
87	1	0	4.127530	2.757798	-5.372980
88	1	0	2.646295	3.673006	-5.034007
89	6	0	4.609960	0.517504	-0.767432
90	6	0	1.416653	0.722418	-0.937497
91	1	0	1.745182	0.270411	0.008749
92	1	0	1.426564	-0.068387	-1.703896
93	28	0	-0.559169	0.660373	-0.671650
94	1	0	0.267533	1.876748	-0.842788
95	5	0	4.323665	0.600077	0.763813
96	8	0	4.930272	-0.223749	1.685376
97	8	0	3.496759	1.523895	1.365042
98	6	0	4.293500	0.012832	2.957964
99	6	0	3.734283	1.459809	2.784144
100	6	0	3.183668	-1.025399	3.100514
101	1	0	2.684040	-0.954652	4.071971
102	1	0	3.617987	-2.024754	3.000443
103	1	0	2.431032	-0.897823	2.315063
104	6	0	5.322346	-0.148190	4.065348
105	1	0	4.887222	0.118667	5.034660
106	1	0	6.198975	0.478286	3.887453
107	1	0	5.649899	-1.190616	4.111728
108	6	0	2.427907	1.734936	3.512766
109	1	0	2.550347	1.595289	4.592813
110	1	0	2.119077	2.768786	3.330819
111	6	0	4.766474	2.537038	3.112524
112	1	0	4.956346	2.596120	4.188550
113	1	0	4.388586	3.503730	2.769205
114	1	0	5.713307	2.338429	2.599769
115	1	0	1.634247	1.073729	3.157314
116	6	0	5.832349	-0.213852	-1.198369
117	6	0	8.156522	-1.586325	-2.009124
118	6	0	7.044664	-0.050036	-0.513865
119	6	0	5.809130	-1.097201	-2.286036
120	6	0	6.956742	-1.773971	-2.690672
121	6	0	8.194329	-0.721291	-0.916855
122	1	0	7.081841	0.613788	0.345421
123	1	0	4.868420	-1.270338	-2.801414
124	1	0	6.911310	-2.453698	-3.536947
125	1	0	9.123778	-0.570310	-0.375669
126	1	0	9.052797	-2.113675	-2.321343

Zero-point correction= 1.048464
(Hartree/Particle)
Thermal correction to Energy= 1.109245
Thermal correction to Enthalpy= 1.110189
Thermal correction to Gibbs Free Energy= 0.950529
Sum of electronic and zero-point Energies= -3401.457855
Sum of electronic and thermal Energies= -3401.397074
Sum of electronic and thermal Enthalpies= -3401.396129
Sum of electronic and thermal Free Energies= -3401.555790

$TS_{VIb\text{-}2B}$

Imaginary frequency: -110.9665

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.994981	1.990131	-4.084139
2	6	0	3.504143	2.194728	-3.136618
3	6	0	2.546379	2.153416	-1.923335
4	6	0	3.443290	1.571617	-0.830515
5	6	0	4.804958	1.331337	-1.439491
6	7	0	4.502325	1.168231	-2.855750
7	1	0	3.986059	3.190564	-3.213566
8	1	0	5.306229	0.442378	-1.035843
9	1	0	5.477257	2.202160	-1.276213
10	6	0	5.670050	1.255744	-3.703881
11	1	0	6.388427	0.473723	-3.435175
12	1	0	5.380585	1.111347	-4.749191
13	6	0	3.047188	1.282593	0.416080
14	28	0	-0.220600	0.527542	-1.126618
15	5	0	-0.082889	2.393462	-0.754179
16	8	0	0.127907	2.679672	0.599236
17	6	0	0.270404	4.098502	0.785834
18	6	0	-0.362722	4.678283	-0.528369
19	8	0	-0.268002	3.583227	-1.454749
20	1	0	2.283755	3.186964	-1.664927
21	6	0	1.242112	1.396809	-2.207562
22	1	0	1.994706	1.429826	0.654761
23	1	0	1.517648	0.418363	-2.630311
24	1	0	0.732880	1.939813	-3.015693
25	6	0	1.757879	4.409213	0.956682
26	1	0	2.138139	3.842416	1.812120
27	1	0	1.919910	5.475271	1.146497
28	1	0	2.342132	4.115159	0.082681
29	6	0	-0.454890	4.498950	2.065112
30	1	0	0.015347	3.998069	2.916776
31	1	0	-1.505451	4.206652	2.043051
32	1	0	-0.390501	5.581730	2.221254
33	6	0	0.383917	5.869433	-1.114771
34	1	0	0.377741	6.714573	-0.417563
35	1	0	-0.106447	6.185434	-2.040269
36	1	0	1.420600	5.614509	-1.347497
37	6	0	-1.842414	5.028534	-0.375835
38	1	0	-2.412005	4.179839	0.017032
39	1	0	-2.251998	5.271807	-1.360393
40	1	0	-1.983662	5.889013	0.286066
41	1	0	6.178657	2.234647	-3.614964
42	1	0	3.262335	-3.630042	2.885296
43	6	0	2.337211	-3.149362	2.584266
44	6	0	0.006461	-1.925162	1.828212
45	6	0	1.447004	-2.697453	3.556123
46	6	0	2.067135	-2.963705	1.231613

47	6	0	0.885176	-2.336892	0.825442
48	6	0	0.258948	-2.064323	3.192920
49	1	0	1.688107	-2.838419	4.604992
50	1	0	2.786087	-3.294360	0.489461
51	6	0	-0.805420	-1.560907	4.165370
52	8	0	-1.175315	-1.360703	1.412534
53	6	0	-1.905607	-2.640875	4.275468
54	1	0	-1.484106	-3.567989	4.677879
55	1	0	-2.340127	-2.855052	3.293017
56	1	0	-2.704973	-2.296989	4.940292
57	6	0	-0.224591	-1.286051	5.551878
58	1	0	0.568208	-0.531569	5.510102
59	1	0	0.184217	-2.202755	5.985597
60	1	0	-1.005912	-0.936693	6.232491
61	6	0	-1.438113	-0.313672	3.551200
62	6	0	-2.788235	1.772327	2.219180
63	6	0	-1.906664	0.796425	4.255268
64	6	0	-1.644432	-0.316318	2.174595
65	6	0	-2.322417	0.685464	1.481220
66	6	0	-2.569612	1.829527	3.594742
67	1	0	-1.760362	0.860968	5.328477
68	1	0	-2.920473	2.688146	4.158532
69	1	0	-3.306739	2.583949	1.717445
70	15	0	0.481858	-1.901882	-0.924405
71	15	0	-2.370160	0.462416	-0.336999
72	6	0	-3.528989	1.748633	-0.948489
73	6	0	-5.304260	3.613835	-2.036229
74	6	0	-3.183627	2.462392	-2.097895
75	6	0	-4.784527	1.956926	-0.361913
76	6	0	-5.659820	2.897617	-0.891746
77	6	0	-4.074630	3.386274	-2.645116
78	1	0	-2.205825	2.310725	-2.546751
79	1	0	-5.077117	1.372315	0.507417
80	1	0	-6.625628	3.062411	-0.424084
81	1	0	-3.797595	3.937027	-3.538869
82	1	0	-5.992918	4.341578	-2.454563
83	6	0	-3.489639	-0.996881	-0.514868
84	6	0	-5.291687	-3.084757	-0.991345
85	6	0	-4.198371	-1.572761	0.541376
86	6	0	-3.680528	-1.488529	-1.810202
87	6	0	-4.583200	-2.518207	-2.049421
88	6	0	-5.091419	-2.616583	0.303287
89	1	0	-4.065009	-1.203857	1.554959
90	1	0	-3.118029	-1.059485	-2.637809
91	1	0	-4.718392	-2.892798	-3.059377
92	1	0	-5.636313	-3.057621	1.132945
93	1	0	-5.991021	-3.894755	-1.176348
94	6	0	1.969421	-2.585139	-1.772429
95	6	0	4.321415	-3.538339	-2.962378
96	6	0	3.042456	-1.724120	-2.017032
97	6	0	2.092018	-3.937417	-2.120764
98	6	0	3.261013	-4.409109	-2.709592
99	6	0	4.208960	-2.195908	-2.616534
100	1	0	2.979590	-0.677515	-1.741624
101	1	0	1.273801	-4.625278	-1.928151
102	1	0	3.344021	-5.459490	-2.972276
103	1	0	5.013904	-1.495441	-2.817684

104	1	0	5.229030	-3.909380	-3.429150
105	6	0	-0.770885	-3.163492	-1.407852
106	6	0	-2.578981	-5.100152	-2.315690
107	6	0	-1.482572	-3.945403	-0.497489
108	6	0	-1.000445	-3.337531	-2.779411
109	6	0	-1.888698	-4.307175	-3.231074
110	6	0	-2.385307	-4.906269	-0.951723
111	1	0	-1.327444	-3.820656	0.570209
112	1	0	-0.454423	-2.730928	-3.499660
113	1	0	-2.041071	-4.444433	-4.297567
114	1	0	-2.935195	-5.506296	-0.232860
115	1	0	-3.275722	-5.855897	-2.666027
116	6	0	3.876139	0.801911	1.534230
117	6	0	5.354219	-0.091954	3.761188
118	6	0	3.255257	0.110139	2.585125
119	6	0	5.252783	1.056294	1.638505
120	6	0	5.983662	0.608427	2.734372
121	6	0	3.984337	-0.334475	3.682388
122	1	0	2.185179	-0.084051	2.529942
123	1	0	5.751246	1.642861	0.874208
124	1	0	7.046944	0.821755	2.793596
125	1	0	3.478182	-0.871026	4.480049
126	1	0	5.923921	-0.433592	4.620082

Zero-point correction=	1.054115
(Hartree/Particle)	
Thermal correction to Energy=	1.113762
Thermal correction to Enthalpy=	1.114706
Thermal correction to Gibbs Free Energy=	0.961179
Sum of electronic and zero-point Energies=	-3401.463575
Sum of electronic and thermal Energies=	-3401.403928
Sum of electronic and thermal Enthalpies=	-3401.402984
Sum of electronic and thermal Free Energies=	-3401.556511

Xb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.752691	-5.399802	-2.299760
2	6	0	2.726331	-4.404787	-1.867461
3	6	0	2.667439	-1.891603	-0.772648
4	6	0	3.842810	-3.576952	-1.973592
5	6	0	1.574060	-3.962920	-1.222787
6	6	0	1.521280	-2.679286	-0.671500
7	6	0	3.834931	-2.298991	-1.417201
8	1	0	4.724477	-3.936044	-2.494487
9	1	0	0.703059	-4.608189	-1.166089
10	6	0	5.007874	-1.323442	-1.416993
11	8	0	2.609219	-0.638726	-0.203127
12	6	0	5.690135	-1.386312	-0.031649
13	1	0	6.090951	-2.390348	0.142524
14	1	0	4.979483	-1.151321	0.766742
15	1	0	6.512845	-0.665029	0.013929
16	6	0	6.036829	-1.657874	-2.495569

17	1	0	5.596310	-1.623973	-3.497150
18	1	0	6.454484	-2.654813	-2.329497
19	1	0	6.872824	-0.953953	-2.456047
20	6	0	4.420287	0.073965	-1.595640
21	6	0	3.221230	2.617335	-1.681929
22	6	0	4.999810	1.108792	-2.328413
23	6	0	3.228158	0.354235	-0.928299
24	6	0	2.601319	1.599126	-0.951969
25	6	0	4.408171	2.370021	-2.367605
26	1	0	5.922910	0.936499	-2.872246
27	1	0	4.876203	3.166006	-2.937650
28	1	0	2.765812	3.602221	-1.724123
29	15	0	0.008440	-1.901638	0.034670
30	15	0	1.010038	1.760337	-0.037058
31	6	0	0.501825	3.450018	-0.542287
32	6	0	-0.472621	5.926667	-1.405527
33	6	0	-0.157986	3.563148	-1.773608
34	6	0	0.668536	4.586324	0.250211
35	6	0	0.173676	5.818945	-0.177612
36	6	0	-0.629804	4.796605	-2.209048
37	1	0	-0.329864	2.672445	-2.375457
38	1	0	1.170014	4.509979	1.210974
39	1	0	0.293091	6.694651	0.453092
40	1	0	-1.133228	4.875578	-3.167926
41	1	0	-0.857044	6.886473	-1.736454
42	6	0	1.604315	1.963227	1.687614
43	6	0	2.386139	2.221900	4.359110
44	6	0	2.864526	2.480536	2.006793
45	6	0	0.742598	1.573422	2.717104
46	6	0	1.131735	1.704090	4.048170
47	6	0	3.252038	2.610143	3.337556
48	1	0	3.542989	2.781477	1.212317
49	1	0	-0.230145	1.154211	2.468951
50	1	0	0.457988	1.387305	4.838319
51	1	0	4.231944	3.011886	3.577401
52	1	0	2.693339	2.318737	5.396069
53	6	0	-1.206312	-3.260821	-0.156366
54	6	0	-3.071239	-5.296721	-0.593244
55	6	0	-1.358170	-4.289691	0.778099
56	6	0	-1.996043	-3.261557	-1.310545
57	6	0	-2.919753	-4.278472	-1.532143
58	6	0	-2.291601	-5.300787	0.561546
59	1	0	-0.747815	-4.299214	1.677006
60	1	0	-1.898055	-2.448390	-2.025850
61	1	0	-3.536959	-4.261551	-2.424583
62	1	0	-2.408627	-6.092390	1.295445
63	1	0	-3.802920	-6.082081	-0.757210
64	6	0	0.325558	-1.901639	1.847564
65	6	0	0.653245	-1.734066	4.624520
66	6	0	1.570586	-2.149702	2.427001
67	6	0	-0.755018	-1.563068	2.674552
68	6	0	-0.596588	-1.492206	4.053750
69	6	0	1.733313	-2.057341	3.809411
70	1	0	2.420061	-2.420871	1.806838
71	1	0	-1.722490	-1.350573	2.223732
72	1	0	-1.445202	-1.237562	4.681879
73	1	0	2.709009	-2.243419	4.247913

74	1	0	0.783573	-1.667407	5.700545
75	28	0	-0.749981	0.280197	-0.204983
76	6	0	-2.588196	2.776511	0.614664
77	1	0	-2.158583	2.870620	1.624334
78	1	0	-2.058399	3.508188	-0.004684
79	6	0	-2.282439	1.391271	0.134466
80	6	0	-2.692837	0.211584	-0.149672
81	7	0	-3.982787	3.196465	0.681348
82	6	0	-4.513082	3.655389	-0.596035
83	1	0	-3.915648	4.517817	-0.921758
84	1	0	-5.532492	4.020235	-0.406548
85	6	0	-4.546317	2.638396	-1.709747
86	1	0	-5.069827	1.704234	-1.505846
87	6	0	-3.980886	2.831051	-2.898751
88	1	0	-4.031454	2.087270	-3.689198
89	1	0	-3.444341	3.750865	-3.123378
90	6	0	-4.845685	2.259098	1.376406
91	1	0	-4.409438	2.035977	2.356712
92	1	0	-4.994910	1.302029	0.853010
93	1	0	-5.824740	2.723569	1.537298
94	1	0	-3.877210	-0.238128	-2.500709
95	6	0	-4.297086	-0.852258	-1.708150
96	6	0	-5.329757	-2.438754	0.326231
97	6	0	-3.775287	-0.720290	-0.409885
98	6	0	-5.324713	-1.749952	-1.978523
99	6	0	-5.846033	-2.550691	-0.963544
100	6	0	-4.310031	-1.533793	0.601448
101	1	0	-5.717097	-1.828420	-2.988723
102	1	0	-6.642905	-3.257070	-1.175317
103	1	0	-3.920883	-1.445097	1.612046
104	1	0	-5.723368	-3.061013	1.124898

Zero-point correction=	0.854984
(Hartree/Particle)	
Thermal correction to Energy=	0.906493
Thermal correction to Enthalpy=	0.907437
Thermal correction to Gibbs Free Energy=	0.768435
Sum of electronic and zero-point Energies=	-2989.932665
Sum of electronic and thermal Energies=	-2989.881156
Sum of electronic and thermal Enthalpies=	-2989.880212
Sum of electronic and thermal Free Energies=	-2990.019215

XIb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.149177	0.043667	-0.716581
2	5	0	-2.182822	-0.061773	-0.432970
3	8	0	-3.169772	-0.032933	-1.411235
4	6	0	-4.462342	-0.261782	-0.808147
5	6	0	-4.199282	0.026823	0.707965
6	8	0	-2.775199	-0.141202	0.824508
7	6	0	-4.526381	1.460957	1.120513
8	1	0	-5.608227	1.628306	1.159564
9	1	0	-4.086316	2.185711	0.432468

10	1	0	-4.107713	1.641564	2.116039
11	6	0	-4.877602	-0.943372	1.668083
12	1	0	-5.966621	-0.911358	1.552147
13	1	0	-4.637970	-0.660617	2.697932
14	1	0	-4.534394	-1.968042	1.507494
15	6	0	-5.478538	0.663000	-1.464811
16	1	0	-6.462014	0.550964	-0.994760
17	1	0	-5.575158	0.400930	-2.523177
18	1	0	-5.172547	1.708904	-1.396237
19	6	0	-4.846762	-1.712831	-1.075687
20	1	0	-5.848467	-1.934819	-0.692650
21	1	0	-4.132223	-2.400966	-0.617096
22	1	0	-4.839389	-1.889443	-2.155008
23	6	0	1.841607	0.218516	-0.886586
24	6	0	2.599389	0.082749	0.225214
25	1	0	2.088080	-0.183879	1.156100
26	6	0	2.478972	0.572607	-2.223394
27	1	0	3.437636	0.045108	-2.343177
28	1	0	2.712377	1.649573	-2.227682
29	7	0	1.716684	0.319680	-3.447929
30	6	0	1.471405	-1.088485	-3.688817
31	1	0	0.691212	-1.492625	-3.021269
32	1	0	2.387813	-1.664550	-3.521626
33	1	0	1.142406	-1.239628	-4.721842
34	6	0	0.496534	1.091671	-3.558317
35	1	0	-0.350905	0.608932	-3.019787
36	1	0	0.651884	2.061776	-3.065788
37	6	0	0.063555	1.349220	-4.980381
38	1	0	-0.945444	1.746881	-5.092058
39	6	0	0.818637	1.142339	-6.055099
40	1	0	0.456597	1.360828	-7.054814
41	1	0	1.826614	0.751168	-5.950612
42	1	0	1.261035	-4.796189	3.681911
43	6	0	0.913141	-3.840815	3.303899
44	6	0	0.068508	-1.390995	2.340487
45	6	0	0.675296	-2.786633	4.184867
46	6	0	0.690343	-3.670035	1.943803
47	6	0	0.257397	-2.440152	1.431832
48	6	0	0.232112	-1.551269	3.721514
49	1	0	0.830600	-2.939414	5.247618
50	1	0	0.870064	-4.493192	1.257520
51	6	0	-0.214426	-0.401452	4.614238
52	8	0	-0.284249	-0.173351	1.834338
53	6	0	-1.759974	-0.454827	4.687672
54	1	0	-2.080820	-1.395890	5.147394
55	1	0	-2.197046	-0.388461	3.685036
56	1	0	-2.134056	0.380974	5.288902
57	6	0	0.359076	-0.501240	6.026723
58	1	0	1.453264	-0.466608	6.023372
59	1	0	0.038105	-1.431246	6.503612
60	1	0	-0.015916	0.314960	6.649999
61	6	0	0.155930	0.904653	3.924319
62	6	0	0.481273	3.309190	2.522796
63	6	0	0.527101	2.070534	4.587629
64	6	0	-0.004223	0.964369	2.535058
65	6	0	0.113561	2.159034	1.812723
66	6	0	0.700974	3.266253	3.893436

67	1	0	0.678818	2.054821	5.661642
68	1	0	0.997893	4.164152	4.424764
69	1	0	0.622824	4.241469	1.983265
70	15	0	-0.027447	-2.209321	-0.371705
71	15	0	-0.182646	2.203082	-0.001723
72	6	0	1.114296	3.392861	-0.565616
73	6	0	3.153422	5.017135	-1.606907
74	6	0	2.409227	3.341100	-0.033040
75	6	0	0.852820	4.283576	-1.612192
76	6	0	1.866993	5.085847	-2.132550
77	6	0	3.418554	4.148482	-0.549563
78	1	0	2.635574	2.659558	0.780338
79	1	0	-0.146693	4.357927	-2.031516
80	1	0	1.645595	5.765846	-2.949290
81	1	0	4.416792	4.086234	-0.126029
82	1	0	3.943649	5.640239	-2.014073
83	6	0	-1.697718	3.221322	-0.234174
84	6	0	-3.956408	4.756674	-0.851376
85	6	0	-2.178689	4.166935	0.676307
86	6	0	-2.365179	3.046269	-1.452087
87	6	0	-3.479047	3.821691	-1.767118
88	6	0	-3.308766	4.922235	0.371755
89	1	0	-1.689926	4.303357	1.635553
90	1	0	-2.024094	2.280156	-2.144878
91	1	0	-3.982400	3.679075	-2.718568
92	1	0	-3.684777	5.641869	1.092376
93	1	0	-4.834042	5.350412	-1.087390
94	6	0	1.353230	-3.227452	-1.072986
95	6	0	3.539951	-4.536332	-2.257411
96	6	0	2.653953	-3.033019	-0.589550
97	6	0	1.163290	-4.111893	-2.139013
98	6	0	2.249395	-4.759315	-2.726892
99	6	0	3.737187	-3.676845	-1.178233
100	1	0	2.828687	-2.370638	0.249565
101	1	0	0.168115	-4.303146	-2.526340
102	1	0	2.079449	-5.440185	-3.555431
103	1	0	4.735278	-3.499763	-0.788371
104	1	0	4.384745	-5.035235	-2.722263
105	6	0	-1.473241	-3.270559	-0.771164
106	6	0	-3.530993	-4.957192	-1.643615
107	6	0	-2.050699	-4.190131	0.107433
108	6	0	-1.968432	-3.172542	-2.078464
109	6	0	-2.969626	-4.031483	-2.521059
110	6	0	-3.085107	-5.019496	-0.325649
111	1	0	-1.696718	-4.263430	1.131059
112	1	0	-1.564290	-2.419625	-2.752914
113	1	0	-3.330809	-3.957386	-3.542257
114	1	0	-3.532194	-5.725097	0.367926
115	1	0	-4.323995	-5.616888	-1.981903
116	1	0	6.998181	1.439420	-0.730272
117	6	0	6.330494	0.849212	-0.108832
118	6	0	4.604629	-0.615369	1.485967
119	6	0	6.846187	0.079810	0.930614
120	6	0	4.960058	0.877972	-0.360344
121	6	0	4.064173	0.130659	0.422270
122	6	0	5.971279	-0.650835	1.734132
123	1	0	7.914855	0.057848	1.120517

124	1	0	4.583742	1.510897	-1.155446
125	1	0	6.355250	-1.245168	2.558484
126	1	0	3.924362	-1.178536	2.124036

Zero-point correction= 1.052822
(Hartree/Particle)
Thermal correction to Energy= 1.113869
Thermal correction to Enthalpy= 1.114813
Thermal correction to Gibbs Free Energy= 0.958839
Sum of electronic and zero-point Energies= -3401.428780
Sum of electronic and thermal Energies= -3401.367733
Sum of electronic and thermal Enthalpies= -3401.366789
Sum of electronic and thermal Free Energies= -3401.522764

$TS_{Xb\text{-}XIb}$

Imaginary frequency: -920.9477

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.308854	0.469502	1.406383
2	5	0	0.959088	1.889529	0.778290
3	8	0	1.606679	2.810066	1.587975
4	6	0	2.622558	3.461927	0.795070
5	6	0	2.075716	3.277411	-0.652411
6	8	0	1.342001	2.040176	-0.541012
7	6	0	1.063254	4.346916	-1.061804
8	1	0	1.542005	5.315923	-1.235000
9	1	0	0.288274	4.469313	-0.296619
10	1	0	0.576101	4.022423	-1.986664
11	6	0	3.147782	3.134187	-1.719483
12	1	0	3.784638	4.026054	-1.743037
13	1	0	2.676746	3.013684	-2.699336
14	1	0	3.771237	2.255692	-1.530988
15	6	0	2.750241	4.907212	1.247608
16	1	0	3.439572	5.454532	0.595045
17	1	0	3.143984	4.941142	2.267603
18	1	0	1.781516	5.412516	1.236732
19	6	0	3.927679	2.704056	1.023602
20	1	0	4.767808	3.185323	0.512381
21	1	0	3.840793	1.673861	0.664489
22	1	0	4.139210	2.677045	2.096746
23	6	0	-2.135136	0.237756	2.186576
24	6	0	-2.005903	1.479070	1.872741
25	1	0	-0.681553	1.945957	1.247445
26	6	0	-3.192599	-0.646224	2.792902
27	1	0	-3.960519	-0.032467	3.285789
28	1	0	-2.743677	-1.287922	3.559259
29	7	0	-3.876144	-1.512989	1.837199
30	6	0	-4.574577	-0.739863	0.822351
31	1	0	-3.899414	-0.093845	0.230537
32	1	0	-5.327419	-0.104338	1.301804
33	1	0	-5.096664	-1.420347	0.144077
34	6	0	-2.984050	-2.503326	1.250406
35	1	0	-2.327230	-2.068275	0.473940
36	1	0	-2.301489	-2.856013	2.034795

37	6	0	-3.707208	-3.698443	0.688025
38	1	0	-3.095030	-4.344813	0.061429
39	6	0	-4.982467	-4.004698	0.914871
40	1	0	-5.434214	-4.896621	0.491222
41	1	0	-5.603795	-3.371231	1.541666
42	1	0	1.126027	1.930988	-5.650094
43	6	0	1.245674	1.336574	-4.749823
44	6	0	1.562842	-0.148258	-2.457759
45	6	0	2.504037	0.849836	-4.404094
46	6	0	0.137620	1.041643	-3.957701
47	6	0	0.280846	0.285472	-2.795385
48	6	0	2.683523	0.085138	-3.250494
49	1	0	3.352548	1.070866	-5.043200
50	1	0	-0.846949	1.403539	-4.240480
51	6	0	3.987216	-0.590023	-2.847462
52	8	0	1.673725	-0.872044	-1.291785
53	6	0	3.927108	-2.055658	-3.337689
54	1	0	3.838370	-2.083111	-4.429016
55	1	0	3.063770	-2.573874	-2.906795
56	1	0	4.834491	-2.592294	-3.040906
57	6	0	5.206159	0.090975	-3.470601
58	1	0	5.293635	1.134872	-3.151052
59	1	0	5.140031	0.064156	-4.561510
60	1	0	6.123884	-0.437885	-3.200354
61	6	0	4.053259	-0.618146	-1.323142
62	6	0	4.040596	-0.969780	1.457214
63	6	0	5.239717	-0.551927	-0.593973
64	6	0	2.864691	-0.829554	-0.616132
65	6	0	2.822311	-1.030687	0.771299
66	6	0	5.234285	-0.725633	0.785807
67	1	0	6.180110	-0.374397	-1.104536
68	1	0	6.163136	-0.669784	1.343810
69	1	0	4.060763	-1.083282	2.534047
70	15	0	-1.093137	-0.216072	-1.677317
71	15	0	1.191387	-1.181074	1.648021
72	6	0	1.706584	-1.220693	3.408859
73	6	0	2.454871	-1.151343	6.105819
74	6	0	1.315686	-0.155922	4.225665
75	6	0	2.479394	-2.253244	3.959376
76	6	0	2.850489	-2.219079	5.298904
77	6	0	1.689513	-0.121332	5.569263
78	1	0	0.715829	0.648762	3.805914
79	1	0	2.788773	-3.088294	3.334944
80	1	0	3.447345	-3.024840	5.714894
81	1	0	1.379291	0.711638	6.192064
82	1	0	2.744030	-1.126831	7.152019
83	6	0	0.599077	-2.900481	1.329030
84	6	0	-0.582655	-5.394809	0.796843
85	6	0	0.385232	-3.326013	0.011301
86	6	0	0.190485	-3.736315	2.375669
87	6	0	-0.385162	-4.977739	2.109703
88	6	0	-0.204269	-4.559095	-0.252136
89	1	0	0.663540	-2.689713	-0.819878
90	1	0	0.303326	-3.419412	3.407086
91	1	0	-0.690936	-5.611747	2.936382
92	1	0	-0.378773	-4.852934	-1.284035
93	1	0	-1.043759	-6.356683	0.593588

94	6	0	-2.389117	1.005608	-2.143765
95	6	0	-4.323025	2.988240	-2.574744
96	6	0	-2.333359	2.223676	-1.453592
97	6	0	-3.417606	0.799837	-3.068518
98	6	0	-4.378364	1.788070	-3.280446
99	6	0	-3.292735	3.209207	-1.662379
100	1	0	-1.530619	2.394226	-0.741079
101	1	0	-3.473778	-0.133697	-3.621151
102	1	0	-5.174399	1.616803	-3.999052
103	1	0	-3.241485	4.136115	-1.096337
104	1	0	-5.082284	3.747848	-2.734097
105	6	0	-1.634183	-1.766761	-2.525878
106	6	0	-2.450534	-4.259051	-3.548716
107	6	0	-0.796445	-2.502618	-3.373179
108	6	0	-2.885850	-2.306087	-2.199124
109	6	0	-3.294853	-3.534144	-2.710013
110	6	0	-1.201191	-3.738721	-3.876866
111	1	0	0.177612	-2.110481	-3.653961
112	1	0	-3.554259	-1.756534	-1.540529
113	1	0	-4.269858	-3.925970	-2.435287
114	1	0	-0.537005	-4.292146	-4.534470
115	1	0	-2.765273	-5.219848	-3.944281
116	1	0	-0.835620	3.931504	1.789297
117	6	0	-2.659762	2.790007	1.843354
118	6	0	-3.960516	5.274883	1.736386
119	6	0	-1.922965	3.979988	1.782642
120	6	0	-4.059150	2.864086	1.857199
121	6	0	-4.701981	4.095911	1.804178
122	6	0	-2.568054	5.211910	1.730280
123	1	0	-4.635949	1.945458	1.886909
124	1	0	-5.787066	4.135155	1.805520
125	1	0	-1.980648	6.124328	1.686941
126	1	0	-4.464628	6.235155	1.689020

Zero-point correction= 1.046986
(Hartree/Particle)
Thermal correction to Energy= 1.108580
Thermal correction to Enthalpy= 1.109524
Thermal correction to Gibbs Free Energy= 0.951009
Sum of electronic and zero-point Energies= -3401.393071
Sum of electronic and thermal Energies= -3401.331476
Sum of electronic and thermal Enthalpies= -3401.330532
Sum of electronic and thermal Free Energies= -3401.489048

Computational results: Chapter 4

- ***Computational methods***

Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the M06-2X hybrid functional[2] that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, N, and O. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set, was used for Ni.[3] Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Gibbs free energy has been used throughout the schemes. The starting approximate geometries for the transition states (TS) were graphically located. Intrinsic reaction coordinate (IRC) studies were performed to confirm the relation of the transition states with the corresponding minima. Solvent effects were considered by performing optimizations in diisopropylether using the polarized continuum model (PCM).

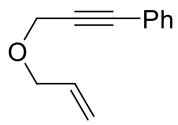
[1] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. 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.

[2] Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, *120,* 215–241.

[3] (a) A. D, Becke, *J. Chem. Phys*. **1993**, *98*, 5648- 5653. (b) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.

- ***Cartesian coordinates and energies of the stationary points***

1a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.089725	-2.994722	1.188470
2	6	0	1.664579	-2.338326	0.077701
3	1	0	2.653612	-1.933794	0.339332
4	1	0	1.810673	-3.103183	-0.691084
5	6	0	1.360035	-2.361552	2.427811
6	1	0	2.446966	-2.304478	2.595609
7	1	0	0.935202	-3.034026	3.180388
8	6	0	0.821375	-1.260337	-0.466592
9	6	0	0.112252	-0.390764	-0.917185
10	6	0	0.755869	-0.991072	2.557515
11	1	0	-0.304670	-0.912616	2.325040
12	6	0	1.445324	0.075346	2.952420
13	1	0	0.977549	1.047502	3.072319
14	1	0	2.507839	0.009858	3.176223
15	6	0	-0.718811	0.664151	-1.422230
16	6	0	-2.339461	2.726562	-2.388470
17	6	0	-0.654866	1.942425	-0.848745
18	6	0	-1.603976	0.429827	-2.483713
19	6	0	-2.408017	1.457948	-2.962198
20	6	0	-1.462171	2.965719	-1.331811
21	1	0	0.031819	2.118253	-0.026612
22	1	0	-1.653928	-0.560765	-2.924020
23	1	0	-3.091915	1.268224	-3.783446
24	1	0	-1.406215	3.952437	-0.882912
25	1	0	-2.968789	3.527383	-2.763809

Zero-point correction= 0.208267
(Hartree/Particle)
Thermal correction to Energy= 0.220492
Thermal correction to Enthalpy= 0.221436
Thermal correction to Gibbs Free Energy= 0.167374
Sum of electronic and zero-point Energies= -539.168476
Sum of electronic and thermal Energies= -539.156250
Sum of electronic and thermal Enthalpies= -539.155306
Sum of electronic and thermal Free Energies= -539.209368

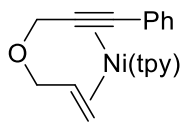
Ni(tpy)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.052871	0.208550	5.683245
2	6	0	0.217690	0.122138	4.635977
3	7	0	0.925991	-0.130110	1.946678

4	6	0	-0.751629	0.179643	3.658524
5	6	0	1.565422	-0.026335	4.257713
6	6	0	1.862425	-0.146341	2.917188
7	6	0	-0.384860	0.068681	2.305220
8	1	0	-1.793774	0.339024	3.914690
9	1	0	2.358445	-0.067172	4.994935
10	1	0	2.883808	-0.292691	2.577916
11	6	0	-1.295071	0.149690	1.185592
12	6	0	-2.642862	-0.173739	-1.203728
13	6	0	-2.642862	-0.173739	1.203728
14	7	0	-0.653762	0.481890	0.000000
15	6	0	-1.295071	0.149690	-1.185592
16	6	0	-3.349303	-0.278484	0.000000
17	1	0	-3.131740	-0.397678	2.147272
18	1	0	-4.398727	-0.548660	0.000000
19	1	0	-3.131740	-0.397678	-2.147272
20	6	0	-0.384860	0.068681	-2.305220
21	6	0	1.565422	-0.026335	-4.257713
22	6	0	-0.751629	0.179643	-3.658524
23	7	0	0.925991	-0.130110	-1.946678
24	6	0	1.862425	-0.146341	-2.917188
25	6	0	0.217690	0.122138	-4.635977
26	1	0	-1.793774	0.339024	-3.914690
27	1	0	2.883808	-0.292691	-2.577916
28	1	0	-0.052871	0.208550	-5.683245
29	1	0	2.358445	-0.067172	-4.994935
30	28	0	1.168782	-0.035608	-0.000000

Zero-point correction= 0.229418
(Hartree/Particle)
Thermal correction to Energy= 0.243551
Thermal correction to Enthalpy= 0.244496
Thermal correction to Gibbs Free Energy= 0.188295
Sum of electronic and zero-point Energies= -911.232594
Sum of electronic and thermal Energies= -911.218461
Sum of electronic and thermal Enthalpies= -911.217517
Sum of electronic and thermal Free Energies= -911.273718

I

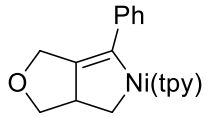


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.637111	0.757347	-0.330960
2	6	0	0.528850	3.583136	1.096053
3	1	0	-0.278600	4.278883	1.344981
4	1	0	1.190060	3.505114	1.976147
5	6	0	0.004206	2.233271	0.784110
6	6	0	-0.722663	1.220766	1.013800
7	6	0	2.232728	3.352481	-0.528436
8	1	0	2.874590	2.917313	0.256066

9	1	0	2.848667	4.026636	-1.135622
10	6	0	1.663075	2.262217	-1.393700
11	1	0	0.917076	2.605664	-2.110836
12	6	0	2.271550	1.040675	-1.595088
13	1	0	2.052836	0.447159	-2.477796
14	1	0	3.177248	0.782785	-1.046404
15	1	0	5.960251	-1.692331	-0.116758
16	6	0	4.986605	-1.412068	0.272494
17	7	0	2.477881	-0.688890	1.261015
18	6	0	3.830779	-2.006047	-0.225173
19	6	0	4.868018	-0.447181	1.266727
20	6	0	3.591951	-0.130324	1.731875
21	6	0	2.599088	-1.597872	0.288094
22	1	0	3.875108	-2.747094	-1.016903
23	1	0	5.739643	0.047219	1.680991
24	1	0	3.457366	0.607977	2.518713
25	6	0	1.330050	-2.158762	-0.255366
26	6	0	-1.038940	-3.131466	-1.193592
27	6	0	1.163847	-3.538486	-0.368787
28	7	0	0.373528	-1.282687	-0.604961
29	6	0	-0.792816	-1.762631	-1.069835
30	6	0	-0.044823	-4.033391	-0.841610
31	1	0	1.966477	-4.201518	-0.064476
32	1	0	-0.208158	-5.102107	-0.934041
33	1	0	-1.992336	-3.470709	-1.583359
34	6	0	-1.840624	-0.777974	-1.459019
35	6	0	-3.701542	1.088823	-2.146953
36	6	0	-3.165538	-0.976984	-1.067618
37	7	0	-1.438691	0.281295	-2.170628
38	6	0	-2.356606	1.189299	-2.499080
39	6	0	-4.111388	-0.020736	-1.416644
40	1	0	-3.432265	-1.830041	-0.451720
41	1	0	-1.999943	2.041647	-3.072695
42	1	0	-5.144435	-0.131546	-1.102373
43	1	0	-4.400566	1.865402	-2.437451
44	1	0	-5.167800	0.827623	2.223314
45	6	0	-4.187697	0.361510	2.171958
46	6	0	-3.103268	1.088874	1.693547
47	1	0	-3.233653	2.112967	1.355817
48	6	0	-1.829935	0.504243	1.606610
49	6	0	-1.674006	-0.825574	2.030817
50	1	0	-0.689207	-1.281126	1.960672
51	6	0	-2.757336	-1.545543	2.523420
52	1	0	-2.616731	-2.571353	2.852458
53	6	0	-4.022007	-0.959819	2.586179
54	1	0	-4.869801	-1.526063	2.959889
55	8	0	1.239587	4.188894	0.032697

Zero-point correction= 0.440534
(Hartree/Particle)
Thermal correction to Energy= 0.467944
Thermal correction to Enthalpy= 0.468889
Thermal correction to Gibbs Free Energy= 0.381288
Sum of electronic and zero-point Energies= -1450.464548
Sum of electronic and thermal Energies= -1450.437138
Sum of electronic and thermal Enthalpies= -1450.436194
Sum of electronic and thermal Free Energies= -1450.523794

II

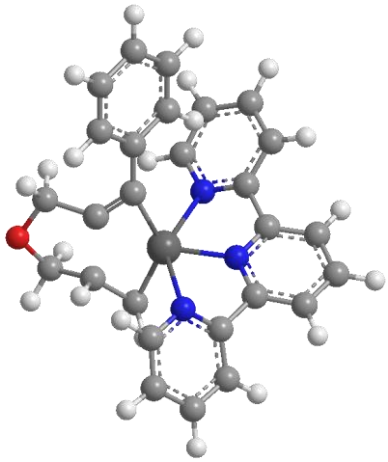


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.738942	5.164181	0.538967
2	6	0	-2.220968	4.210846	0.550160
3	7	0	-0.900498	1.772025	0.540799
4	6	0	-0.947948	4.102020	-0.001845
5	6	0	-2.802904	3.093452	1.132832
6	6	0	-2.107275	1.887924	1.096236
7	6	0	-0.306564	2.866801	0.029740
8	1	0	-0.465011	4.971981	-0.429413
9	1	0	-3.780950	3.137813	1.597153
10	1	0	-2.530217	0.981507	1.512420
11	6	0	1.112150	2.674702	-0.374375
12	6	0	3.790465	2.253155	-0.689202
13	6	0	1.897646	3.702047	-0.892274
14	7	0	1.616010	1.456244	-0.102205
15	6	0	2.938087	1.261638	-0.196036
16	6	0	3.255348	3.472949	-1.075788
17	1	0	1.468073	4.666356	-1.132994
18	1	0	3.894537	4.253850	-1.473829
19	1	0	4.858274	2.072987	-0.735434
20	6	0	3.493535	-0.018872	0.318719
21	6	0	4.426732	-2.381406	1.302420
22	6	0	4.581760	-0.624217	-0.311761
23	7	0	2.899151	-0.527606	1.403757
24	6	0	3.362480	-1.684168	1.874432
25	6	0	5.051650	-1.832907	0.189376
26	1	0	5.021207	-0.182430	-1.199705
27	1	0	2.859229	-2.075833	2.755097
28	1	0	5.882114	-2.340856	-0.289970
29	1	0	4.752275	-3.325048	1.725667
30	28	0	0.078925	0.052198	-0.054479
31	1	0	0.620045	-1.403888	-2.002745
32	6	0	0.972439	-1.453034	-0.960069
33	1	0	2.067106	-1.442622	-0.981446
34	6	0	0.413494	-2.727288	-0.330825
35	6	0	0.322267	-4.010460	-1.163102
36	6	0	-1.779788	-3.787603	-0.230189
37	6	0	-1.049149	-2.468190	-0.094005
38	1	0	0.934608	-2.956688	0.612752
39	1	0	0.134301	-3.753684	-2.219481
40	1	0	1.198542	-4.663263	-1.110003
41	1	0	-2.585083	-3.727064	-0.979947
42	1	0	-2.222268	-4.153290	0.704052
43	6	0	-1.462477	-1.191112	-0.060147
44	8	0	-0.784371	-4.733651	-0.626432
45	1	0	-2.727048	0.520471	-1.689150
46	1	0	-6.709417	0.039676	-0.134508
47	6	0	-5.654599	-0.217266	-0.118867
48	6	0	-2.906716	-0.880422	-0.071701

49	6	0	-5.166915	-1.134228	0.810107
50	6	0	-4.772108	0.367973	-1.027812
51	6	0	-3.419702	0.046729	-0.996062
52	6	0	-3.812387	-1.462679	0.829985
53	1	0	-5.843836	-1.594680	1.524593
54	1	0	-5.141161	1.082840	-1.758230
55	1	0	-3.435288	-2.167597	1.566882

Zero-point correction= 0.443910
(Hartree/Particle)
Thermal correction to Energy= 0.469942
Thermal correction to Enthalpy= 0.470886
Thermal correction to Gibbs Free Energy= 0.386366
Sum of electronic and zero-point Energies= -1450.493167
Sum of electronic and thermal Energies= -1450.467136
Sum of electronic and thermal Enthalpies= -1450.466192
Sum of electronic and thermal Free Energies= -1450.550712

TS(I-II)



Imaginary frequency: -63.7139 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.864337	3.980131	0.779464
2	6	0	3.058431	3.298972	1.033311
3	7	0	0.990265	1.541435	1.659540
4	6	0	1.815709	3.421850	0.421153
5	6	0	3.253817	2.278925	1.957552
6	6	0	2.187079	1.425060	2.231306
7	6	0	0.806787	2.518119	0.766113
8	1	0	1.642312	4.182803	-0.332003
9	1	0	4.208817	2.138579	2.451128
10	1	0	2.296382	0.609329	2.941756
11	6	0	-0.541040	2.606218	0.135913
12	6	0	-3.022446	2.733590	-1.006835
13	6	0	-1.075459	3.851658	-0.199824
14	7	0	-1.215234	1.462447	-0.075339
15	6	0	-2.436723	1.524073	-0.634109
16	6	0	-2.331590	3.916190	-0.783835
17	1	0	-0.516512	4.753702	0.020301
18	1	0	-2.766245	4.871888	-1.057656

19	1	0	-3.998368	2.733992	-1.479242
20	6	0	-3.172285	0.244855	-0.844939
21	6	0	-4.440211	-2.147146	-1.182191
22	6	0	-4.538247	0.164727	-0.567489
23	7	0	-2.458844	-0.796104	-1.282800
24	6	0	-3.083813	-1.960137	-1.445645
25	6	0	-5.179631	-1.058357	-0.735755
26	1	0	-5.076035	1.030411	-0.195079
27	1	0	-2.467957	-2.782834	-1.801598
28	1	0	-6.236834	-1.159217	-0.511961
29	1	0	-4.896086	-3.120692	-1.323662
30	28	0	-0.460136	-0.325089	0.477502
31	1	0	-1.498753	-0.749691	2.835366
32	6	0	-1.636290	-1.100216	1.810437
33	1	0	-2.683896	-1.187175	1.521757
34	6	0	-0.777457	-2.245118	1.423953
35	6	0	0.784908	-2.013910	0.487033
36	1	0	-1.275618	-2.937922	0.739497
37	6	0	1.109552	-1.093696	-0.399078
38	1	0	2.235513	-3.010685	-1.961556
39	6	0	-0.116665	-3.007386	2.556135
40	6	0	1.614612	-3.126017	1.097525
41	1	0	0.342991	-2.294359	3.261912
42	1	0	-0.843490	-3.619976	3.095403
43	1	0	2.478685	-2.672660	1.611836
44	1	0	1.997350	-3.812107	0.337028
45	1	0	2.697948	1.041913	-0.657207
46	6	0	3.071385	0.188930	-1.217039
47	6	0	2.333195	-1.005208	-1.188478
48	6	0	2.808277	-2.086966	-1.949173
49	6	0	3.978799	-1.982502	-2.693402
50	1	0	4.320879	-2.831577	-3.278659
51	6	0	4.714054	-0.797903	-2.688153
52	1	0	5.630403	-0.718933	-3.265152
53	6	0	4.253388	0.286672	-1.942769
54	1	0	4.812402	1.218667	-1.936758
55	8	0	0.846680	-3.878401	2.009361

Zero-point correction= 0.440527
(Hartree/Particle)
Thermal correction to Energy= 0.466992
Thermal correction to Enthalpy= 0.467936
Thermal correction to Gibbs Free Energy= 0.381927
Sum of electronic and zero-point Energies= -1450.437558
Sum of electronic and thermal Energies= -1450.411093
Sum of electronic and thermal Enthalpies= -1450.410149
Sum of electronic and thermal Free Energies= -1450.496159

TS(I-II)t

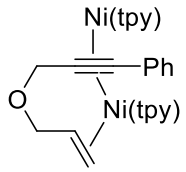
Imaginary frequency: -216.0509

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.419204	5.856881	0.106884
2	6	0	0.326972	4.781067	0.215015
3	7	0	0.084314	2.036462	0.477343
4	6	0	-0.830852	4.134803	-0.205298
5	6	0	1.364153	4.032900	0.760708
6	6	0	1.197098	2.654812	0.865204
7	6	0	-0.919418	2.750863	-0.055059
8	1	0	-1.639047	4.700716	-0.653958
9	1	0	2.285553	4.498239	1.091240
10	1	0	1.976306	2.007607	1.260883
11	6	0	-2.107001	1.958155	-0.488758
12	6	0	-4.157620	0.284425	-1.230526
13	6	0	-3.306859	2.517985	-0.930537
14	7	0	-1.950553	0.634173	-0.423227
15	6	0	-2.929278	-0.201303	-0.778723
16	6	0	-4.337317	1.661418	-1.302664
17	1	0	-3.447283	3.591340	-0.972582
18	1	0	-5.283616	2.067460	-1.644285
19	1	0	-4.961481	-0.386932	-1.507677
20	6	0	-2.594684	-1.649928	-0.651680
21	6	0	-1.783758	-4.255031	-0.380991
22	6	0	-3.414269	-2.666370	-1.142077
23	7	0	-1.423795	-1.917843	-0.054281
24	6	0	-1.021484	-3.179982	0.068393
25	6	0	-3.001716	-3.986523	-0.995843
26	1	0	-4.348416	-2.439751	-1.642751
27	1	0	-0.046120	-3.311491	0.530837
28	1	0	-3.622082	-4.794627	-1.369614
29	1	0	-1.422690	-5.269625	-0.258917
30	28	0	-0.243201	-0.146619	0.545905
31	1	0	-1.018109	0.820773	2.989324
32	6	0	-1.018332	-0.208881	2.638830
33	1	0	-1.982475	-0.672874	2.458396
34	6	0	0.136803	-0.988845	2.754743
35	6	0	1.740346	-0.982781	1.134053
36	1	0	0.017652	-2.069026	2.675501
37	6	0	1.628136	-0.781492	-0.155198
38	1	0	3.717872	-2.419252	-0.698525
39	6	0	1.251826	-0.576235	3.682812
40	6	0	2.884685	-0.984832	2.098237
41	1	0	1.386313	0.519803	3.628377
42	1	0	0.981028	-0.831496	4.713493
43	1	0	3.400491	-0.005722	2.081718
44	1	0	3.628285	-1.752487	1.857777
45	1	0	1.770187	1.168214	-1.999329
46	6	0	2.582170	0.451009	-2.100750
47	6	0	2.630794	-0.630840	-1.202109
48	6	0	3.668871	-1.567377	-1.372303
49	6	0	4.612335	-1.423668	-2.384050
50	1	0	5.398943	-2.165712	-2.494270
51	6	0	4.560281	-0.332101	-3.250292

52	1	0	5.299732	-0.217707	-4.036899
53	6	0	3.539166	0.606722	-3.096794
54	1	0	3.483396	1.460238	-3.767635
55	8	0	2.454992	-1.253327	3.425219

Zero-point correction= 0.438475
(Hartree/Particle)
Thermal correction to Energy= 0.465515
Thermal correction to Enthalpy= 0.466459
Thermal correction to Gibbs Free Energy= 0.378052
Sum of electronic and zero-point Energies= -1450.444454
Sum of electronic and thermal Energies= -1450.417414
Sum of electronic and thermal Enthalpies= -1450.416470
Sum of electronic and thermal Free Energies= -1450.504877

III



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.678714	-3.500491	-0.396175
2	6	0	0.878335	-2.276960	-1.099637
3	1	0	1.259037	-2.522726	-2.105063
4	1	0	1.655593	-1.687790	-0.597654
5	6	0	-0.336300	-1.439791	-1.239699
6	6	0	-1.635145	-1.372505	-1.198361
7	6	0	1.521131	-3.638361	0.742159
8	1	0	2.555494	-3.384180	0.459869
9	1	0	1.511108	-4.718368	0.953469
10	6	0	1.086669	-2.846866	1.959353
11	1	0	1.890220	-2.777410	2.702712
12	6	0	-0.268461	-3.005186	2.424057
13	1	0	-0.477110	-3.028595	3.497374
14	1	0	-0.953923	-3.617257	1.831566
15	28	0	-0.843514	0.335599	-1.521244
16	1	0	4.786419	-2.040321	-3.171427
17	6	0	3.857469	-1.495871	-3.311711
18	7	0	1.470538	-0.087804	-3.659661
19	6	0	3.543179	-0.417250	-2.493556
20	6	0	2.957929	-1.863556	-4.305751
21	6	0	1.782593	-1.124373	-4.436168
22	6	0	2.334255	0.251470	-2.696658
23	1	0	4.205679	-0.106366	-1.694594
24	1	0	3.155396	-2.698984	-4.968215
25	1	0	1.057603	-1.375824	-5.206384
26	6	0	1.991571	1.456490	-1.890122
27	6	0	1.287320	3.827701	-0.704787
28	6	0	2.992788	2.355827	-1.511378
29	7	0	0.701045	1.698333	-1.632572
30	6	0	0.345242	2.879817	-1.098159
31	6	0	2.634311	3.542445	-0.890085

32	1	0	4.030522	2.138093	-1.735516
33	1	0	3.392629	4.255448	-0.582793
34	1	0	0.984017	4.766253	-0.256908
35	6	0	-1.122667	3.116956	-1.023026
36	6	0	-3.844858	3.436164	-1.134525
37	6	0	-1.678368	4.344083	-0.659230
38	7	0	-1.890989	2.078365	-1.404600
39	6	0	-3.214413	2.239494	-1.460675
40	6	0	-3.058862	4.503958	-0.717044
41	1	0	-1.048557	5.172626	-0.357915
42	1	0	-3.780997	1.371917	-1.778531
43	1	0	-3.509780	5.454230	-0.449694
44	1	0	-4.923245	3.519046	-1.206973
45	28	0	-0.002260	-1.212459	1.807338
46	1	0	5.490805	-1.283987	3.799802
47	6	0	4.868052	-1.055354	2.940834
48	7	0	3.247204	-0.467047	0.738699
49	6	0	3.879339	-0.080951	3.023982
50	6	0	5.032527	-1.733932	1.739542
51	6	0	4.200970	-1.395907	0.674006
52	6	0	3.084687	0.166094	1.901943
53	1	0	3.701487	0.463342	3.945789
54	1	0	5.784104	-2.506498	1.622309
55	1	0	4.303934	-1.902970	-0.284180
56	6	0	2.005023	1.191182	2.002542
57	6	0	0.010286	3.015012	2.391873
58	6	0	2.337938	2.489186	2.396478
59	7	0	0.739326	0.801273	1.793270
60	6	0	-0.245606	1.698269	2.003870
61	6	0	1.323658	3.417553	2.586158
62	1	0	3.379566	2.749096	2.552351
63	1	0	1.550465	4.432749	2.896241
64	1	0	-0.807754	3.700717	2.579498
65	6	0	-1.633923	1.177934	1.905533
66	6	0	-4.116133	0.029786	1.796691
67	6	0	-2.753914	2.001461	1.827114
68	7	0	-1.737678	-0.160531	1.939433
69	6	0	-2.945494	-0.721230	1.884429
70	6	0	-4.014207	1.414064	1.768677
71	1	0	-2.651044	3.079590	1.780440
72	1	0	-2.965342	-1.806929	1.901137
73	1	0	-4.901264	2.035799	1.695181
74	1	0	-5.074332	-0.473855	1.739517
75	1	0	-5.842990	-4.473448	0.014407
76	6	0	-4.993611	-3.849859	-0.248456
77	6	0	-2.783919	-2.223481	-0.916320
78	6	0	-3.691753	-4.339697	-0.123624
79	6	0	-5.191488	-2.553257	-0.720070
80	6	0	-4.099028	-1.754410	-1.048114
81	6	0	-2.602093	-3.542497	-0.457680
82	1	0	-3.526604	-5.350615	0.239825
83	1	0	-6.199738	-2.162095	-0.829653
84	1	0	-4.252874	-0.737947	-1.399619
85	1	0	-1.582865	-3.906782	-0.356015

Zero-point correction= 0.674107
(Hartree/Particle)

Thermal correction to Energy= 0.716697
Thermal correction to Enthalpy= 0.717641
Thermal correction to Gibbs Free Energy= 0.598489
Sum of electronic and zero-point Energies= -2361.746327
Sum of electronic and thermal Energies= -2361.703738
Sum of electronic and thermal Enthalpies= -2361.702793
Sum of electronic and thermal Free Energies= -2361.821946

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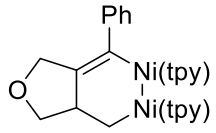


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.001065	5.571224	0.883237
2	6	0	-1.815372	4.502911	0.831552
3	7	0	-1.355838	1.746798	0.707274
4	6	0	-0.640121	3.978385	1.319613
5	6	0	-2.770921	3.635361	0.267854
6	6	0	-2.488034	2.285516	0.224246
7	6	0	-0.408063	2.591908	1.253097
8	1	0	0.119787	4.624813	1.747490
9	1	0	-3.708977	4.003728	-0.129838
10	1	0	-3.191737	1.582656	-0.207478
11	6	0	0.759562	1.927595	1.758809
12	6	0	2.721136	0.241975	2.805926
13	6	0	1.834933	2.476757	2.473587
14	7	0	0.718194	0.573623	1.568646
15	6	0	1.633249	-0.250858	2.115440
16	6	0	2.820990	1.646387	2.972636
17	1	0	1.895176	3.549133	2.632181
18	1	0	3.657955	2.065984	3.519939
19	1	0	3.459038	-0.420633	3.244332
20	6	0	1.276851	-1.668998	1.934530
21	6	0	0.336278	-4.230887	1.619053
22	6	0	2.048824	-2.739047	2.385644
23	7	0	0.080479	-1.869913	1.317730
24	6	0	-0.375738	-3.122374	1.182517
25	6	0	1.576796	-4.033271	2.225568
26	1	0	3.006317	-2.552586	2.858861
27	1	0	-1.349012	-3.213102	0.709964
28	1	0	2.165023	-4.877277	2.571147
29	1	0	-0.080105	-5.222531	1.486920
30	28	0	-0.831206	-0.164683	0.739762
31	1	0	-0.957733	-0.526852	-3.288539
32	6	0	-0.316083	-1.161923	-2.662327
33	1	0	0.325818	-1.711552	-3.377759
34	6	0	-1.200186	-2.196462	-1.962120
35	6	0	-1.836465	-3.191730	-2.948832
36	6	0	-3.593803	-2.535766	-1.722737
37	6	0	-2.422595	-1.729595	-1.168043
38	1	0	-0.585650	-2.784134	-1.265288
39	1	0	-2.099184	-2.666367	-3.884024

40	1	0	-1.192916	-4.041685	-3.197271
41	1	0	-4.149723	-1.971678	-2.492773
42	1	0	-4.305233	-2.862841	-0.959283
43	6	0	-2.427579	-0.946249	-0.074417
44	1	0	-4.807430	-0.562195	3.897496
45	1	0	4.886453	-4.143964	0.091611
46	6	0	4.156934	-3.426209	-0.269015
47	7	0	2.268869	-1.582707	-1.182120
48	6	0	4.343432	-2.070690	-0.058565
49	6	0	3.020327	-3.850229	-0.965203
50	6	0	2.113571	-2.898977	-1.398577
51	6	0	3.388417	-1.164426	-0.525772
52	1	0	5.216740	-1.704332	0.470051
53	1	0	2.836398	-4.899041	-1.166339
54	1	0	1.228379	-3.185399	-1.954271
55	6	0	3.497644	0.293110	-0.387091
56	6	0	3.358898	3.046900	-0.352240
57	6	0	4.567964	0.996890	0.124484
58	7	0	2.404178	0.925653	-0.859656
59	6	0	2.304454	2.281437	-0.862364
60	6	0	4.476582	2.404293	0.160502
61	1	0	5.449959	0.491720	0.501647
62	1	0	5.300613	2.987071	0.558110
63	1	0	3.300896	4.130549	-0.344723
64	6	0	1.084865	2.746764	-1.477729
65	6	0	-1.294182	3.413237	-2.702375
66	6	0	0.741138	4.101874	-1.639557
67	7	0	0.263666	1.747158	-1.950167
68	6	0	-0.895311	2.102554	-2.527342
69	6	0	-0.442258	4.440196	-2.252903
70	1	0	1.409807	4.869373	-1.263556
71	1	0	-1.530545	1.283157	-2.845226
72	1	0	-0.718160	5.482494	-2.377708
73	1	0	-2.241355	3.628736	-3.182024
74	28	0	0.990282	-0.094102	-1.660914
75	8	0	-3.007294	-3.682411	-2.321528
76	6	0	-4.844594	-0.523740	2.812363
77	6	0	-4.914531	-0.424483	0.038835
78	6	0	-6.048023	-0.244723	2.164931
79	6	0	-3.686234	-0.742705	2.074229
80	6	0	-3.692281	-0.715977	0.668251
81	6	0	-6.074944	-0.191537	0.773455
82	1	0	-6.951345	-0.061688	2.738710
83	1	0	-2.747169	-0.942374	2.587699
84	1	0	-7.002306	0.037174	0.255713
85	1	0	-4.944485	-0.355742	-1.045968

Zero-point correction= 0.676263
(Hartree/Particle)
Thermal correction to Energy= 0.716654
Thermal correction to Enthalpy= 0.717598
Thermal correction to Gibbs Free Energy= 0.606200
Sum of electronic and zero-point Energies= -2361.828571
Sum of electronic and thermal Energies= -2361.788180
Sum of electronic and thermal Enthalpies= -2361.787236
Sum of electronic and thermal Free Energies= -2361.898634

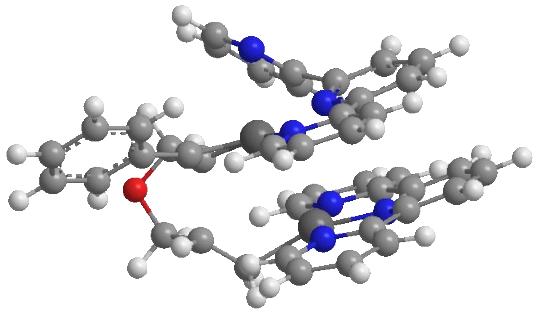
23t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.994536	5.225410	2.003385
2	6	0	-0.946785	4.161803	1.790124
3	7	0	-0.839631	1.424804	1.215479
4	6	0	0.176068	3.440863	2.110448
5	6	0	-2.036373	3.505094	1.171200
6	6	0	-1.922411	2.158614	0.899905
7	6	0	0.224554	2.053051	1.838157
8	1	0	1.031964	3.919634	2.575024
9	1	0	-2.938328	4.038510	0.896184
10	1	0	-2.724780	1.616156	0.410870
11	6	0	1.316499	1.194003	2.163563
12	6	0	3.172746	-0.827365	2.691146
13	6	0	2.496014	1.499927	2.874543
14	7	0	1.124364	-0.091622	1.736699
15	6	0	2.001080	-1.074380	2.009300
16	6	0	3.413837	0.503106	3.126536
17	1	0	2.676227	2.511411	3.224206
18	1	0	4.322200	0.730406	3.674402
19	1	0	3.882195	-1.617704	2.905874
20	6	0	1.514531	-2.388383	1.539687
21	6	0	0.360620	-4.743277	0.726459
22	6	0	2.236007	-3.574166	1.654860
23	7	0	0.261724	-2.371637	1.016713
24	6	0	-0.298902	-3.524271	0.633145
25	6	0	1.654325	-4.764350	1.240638
26	1	0	3.242119	-3.557096	2.057714
27	1	0	-1.308038	-3.443965	0.239675
28	1	0	2.202198	-5.697740	1.320338
29	1	0	-0.136884	-5.649678	0.402186
30	28	0	-0.533258	-0.511019	0.878914
31	1	0	-1.352423	-0.196914	-3.422634
32	6	0	-0.613453	-0.807297	-2.881682
33	1	0	0.010965	-1.267155	-3.669037
34	6	0	-1.353494	-1.930660	-2.154404
35	6	0	-2.129590	-2.851374	-3.119451
36	6	0	-3.718740	-2.176031	-1.685712
37	6	0	-2.440593	-1.542517	-1.150900
38	1	0	-0.617387	-2.542785	-1.619005
39	1	0	-2.441866	-2.275042	-4.007513
40	1	0	-1.557853	-3.722399	-3.453616
41	1	0	-4.264879	-1.496072	-2.365243
42	1	0	-4.408166	-2.510892	-0.906666
43	6	0	-2.260696	-0.975152	0.056009
44	1	0	-4.295064	-1.122686	4.235413
45	1	0	5.053562	-3.327547	-0.659805
46	6	0	4.221390	-2.679262	-0.917089
47	7	0	2.046343	-1.029472	-1.562469
48	6	0	4.248342	-1.350587	-0.579168
49	6	0	3.097590	-3.192490	-1.609776
50	6	0	2.059958	-2.332693	-1.897190
51	6	0	3.161080	-0.507775	-0.918849
52	1	0	5.097261	-0.927997	-0.051017

53	1	0	3.037931	-4.232770	-1.906153
54	1	0	1.185969	-2.686012	-2.434355
55	6	0	3.104677	0.891019	-0.654095
56	6	0	2.622595	3.637226	-0.402441
57	6	0	4.097459	1.727281	-0.090774
58	7	0	1.924983	1.459822	-1.044020
59	6	0	1.688646	2.774696	-0.938647
60	6	0	3.854325	3.076720	0.031636
61	1	0	5.041566	1.309067	0.243304
62	1	0	4.612018	3.724433	0.460637
63	1	0	2.435326	4.700455	-0.313415
64	6	0	0.347943	3.132955	-1.456709
65	6	0	-2.182956	3.581871	-2.417553
66	6	0	-0.151093	4.432596	-1.479032
67	7	0	-0.378768	2.086714	-1.927859
68	6	0	-1.619245	2.312581	-2.369942
69	6	0	-1.426250	4.662858	-1.977728
70	1	0	0.453625	5.249692	-1.102817
71	1	0	-2.174726	1.437577	-2.688310
72	1	0	-1.829192	5.670056	-2.006807
73	1	0	-3.190809	3.709383	-2.794669
74	28	0	0.616027	0.317541	-1.866728
75	8	0	-3.272695	-3.309577	-2.417547
76	6	0	-4.400258	-0.871173	3.183774
77	6	0	-4.647167	-0.231435	0.494040
78	6	0	-5.603011	-0.348181	2.708833
79	6	0	-3.329116	-1.064371	2.317557
80	6	0	-3.428605	-0.765289	0.947397
81	6	0	-5.719210	-0.025469	1.358988
82	1	0	-6.436277	-0.187697	3.386018
83	1	0	-2.390022	-1.461793	2.699508
84	1	0	-6.646908	0.391743	0.977318
85	1	0	-4.740102	0.043847	-0.554479

Zero-point correction= 0.675799
(Hartree/Particle)
Thermal correction to Energy= 0.716411
Thermal correction to Enthalpy= 0.717355
Thermal correction to Gibbs Free Energy= 0.604388
Sum of electronic and zero-point Energies= -2361.832154
Sum of electronic and thermal Energies= -2361.791542
Sum of electronic and thermal Enthalpies= -2361.790597
Sum of electronic and thermal Free Energies= -2361.903565

TS(III-23)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	1	0	-2.272013	-3.486971	-0.793127
4	1	0	-0.708916	-3.567177	0.063042
5	6	0	-1.662486	-1.625744	0.124686
6	6	0	-2.645859	-0.755784	-0.159311
7	6	0	-1.798452	-3.031649	2.341560
8	1	0	-0.811269	-3.492280	2.507692
9	1	0	-2.421236	-3.250844	3.216632
10	6	0	-1.622461	-1.522918	2.234532
11	1	0	-2.557780	-0.970736	2.294045
12	6	0	-0.492932	-0.955276	2.882433
13	1	0	-0.699664	-0.102807	3.531207
14	1	0	0.182128	-1.679774	3.344755
15	28	0	-1.065024	0.050686	-0.692519
16	1	0	2.339282	-5.163539	-1.321154
17	6	0	1.700488	-4.365304	-1.687829
18	7	0	0.064072	-2.296250	-2.603908
19	6	0	2.074084	-3.036265	-1.520925
20	6	0	0.502816	-4.646240	-2.334279
21	6	0	-0.274180	-3.573483	-2.770868
22	6	0	1.223485	-2.033967	-1.986691
23	1	0	3.006806	-2.770522	-1.034771
24	1	0	0.170903	-5.665531	-2.499104
25	1	0	-1.217618	-3.751435	-3.282542
26	6	0	1.643663	-0.601595	-1.967419
27	6	0	2.228560	2.026096	-2.458440
28	6	0	2.891145	-0.272205	-2.488410
29	7	0	0.749007	0.329166	-1.599254
30	6	0	1.014444	1.634440	-1.871674
31	6	0	3.182740	1.074354	-2.740573
32	1	0	3.575505	-1.060601	-2.781676
33	1	0	4.135400	1.362274	-3.173591
34	1	0	2.422298	3.069722	-2.674761
35	6	0	-0.088288	2.563274	-1.616553
36	6	0	-2.307791	4.130874	-1.144067
37	6	0	-0.031768	3.938958	-1.883818
38	7	0	-1.223970	1.993453	-1.142875
39	6	0	-2.286214	2.771920	-0.890541
40	6	0	-1.145080	4.724763	-1.648159
41	1	0	0.880471	4.386978	-2.260770
42	1	0	-3.147383	2.265013	-0.466826

43	1	0	-1.113133	5.789934	-1.854833
44	1	0	-3.196731	4.711376	-0.926875
45	28	0	0.899102	0.051770	1.708453
46	1	0	5.255616	-3.846396	1.154998
47	6	0	4.408993	-3.169649	1.205482
48	7	0	2.230434	-1.420978	1.378689
49	6	0	4.560467	-1.834092	0.888575
50	6	0	3.141029	-3.634005	1.596406
51	6	0	2.099586	-2.730131	1.660626
52	6	0	3.459277	-0.967421	0.974814
53	1	0	5.526168	-1.438510	0.592381
54	1	0	2.966571	-4.676106	1.837253
55	1	0	1.102433	-3.049786	1.939875
56	6	0	3.506403	0.464390	0.732002
57	6	0	3.171891	3.179315	0.317072
58	6	0	4.536827	1.176848	0.163637
59	7	0	2.373633	1.089281	1.169495
60	6	0	2.151154	2.421820	0.897071
61	6	0	4.364268	2.565974	-0.046110
62	1	0	5.447106	0.681478	-0.158166
63	1	0	5.156944	3.144934	-0.507473
64	1	0	3.017253	4.236101	0.117291
65	6	0	0.858793	2.857553	1.318599
66	6	0	-1.682304	3.448166	2.243988
67	6	0	0.442558	4.208061	1.419487
68	7	0	0.012849	1.834173	1.699667
69	6	0	-1.218125	2.155824	2.143632
70	6	0	-0.811965	4.504781	1.881110
71	1	0	1.134822	4.997237	1.143844
72	1	0	-1.855957	1.314432	2.399867
73	1	0	-1.138715	5.537098	1.960099
74	1	0	-2.688830	3.636782	2.598088
75	1	0	-7.986520	-0.668503	-0.343433
76	6	0	-6.901553	-0.691358	-0.307019
77	6	0	-4.094326	-0.745427	-0.207573
78	6	0	-6.249296	-1.583039	0.542901
79	6	0	-6.157374	0.163785	-1.121219
80	6	0	-4.769735	0.145631	-1.062046
81	6	0	-4.859669	-1.623077	0.584596
82	1	0	-6.827809	-2.259867	1.164667
83	1	0	-6.662240	0.846026	-1.798613
84	1	0	-4.180372	0.797443	-1.700864
85	1	0	-4.343920	-2.345879	1.209637

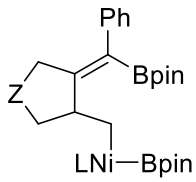
Zero-point correction=	0.671886
(Hartree/Particle)	
Thermal correction to Energy=	0.713031
Thermal correction to Enthalpy=	0.713975
Thermal correction to Gibbs Free Energy=	0.600784
Sum of electronic and zero-point Energies=	-2361.705851
Sum of electronic and thermal Energies=	-2361.664707
Sum of electronic and thermal Enthalpies=	-2361.663762
Sum of electronic and thermal Free Energies=	-2361.776954

B_2pin_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000125	0.852027	-0.001050
2	8	0	0.100439	1.615030	-1.137007
3	6	0	0.298374	2.986669	-0.720931
4	6	0	-0.298388	2.985944	0.721065
5	8	0	-0.100583	1.613844	1.135693
6	5	0	0.000125	-0.852027	-0.001050
7	8	0	-0.100439	-1.615030	-1.137007
8	6	0	-0.298374	-2.986669	-0.720931
9	6	0	0.298388	-2.985944	0.721065
10	8	0	0.100583	-1.613844	1.135693
11	6	0	0.405252	3.907205	1.704134
12	1	0	1.457602	3.640002	1.818762
13	1	0	-0.076157	3.833644	2.683333
14	1	0	0.340033	4.947177	1.366772
15	6	0	1.804808	-3.238776	0.741546
16	1	0	2.320925	-2.582205	0.034006
17	1	0	2.038545	-4.277736	0.490837
18	1	0	2.184202	-3.027700	1.744952
19	6	0	-0.405252	-3.907205	1.704134
20	1	0	-0.340033	-4.947177	1.366772
21	1	0	-1.457602	-3.640002	1.818762
22	1	0	0.076157	-3.833644	2.683333
23	6	0	-1.804808	3.238776	0.741546
24	1	0	-2.320925	2.582205	0.034006
25	1	0	-2.038545	4.277736	0.490837
26	1	0	-2.184202	3.027700	1.744952
27	6	0	-0.405051	3.909099	-1.703077
28	1	0	0.076617	3.836902	-2.682248
29	1	0	-0.340004	4.948633	-1.364339
30	1	0	-1.457349	3.641958	-1.818314
31	6	0	1.804808	3.239342	-0.741058
32	1	0	2.184245	3.029086	-1.744610
33	1	0	2.320820	2.582131	-0.034029
34	1	0	2.038580	4.278077	-0.489439
35	6	0	-1.804808	-3.239342	-0.741058
36	1	0	-2.184245	-3.029086	-1.744610
37	1	0	-2.320820	-2.582131	-0.034029
38	1	0	-2.038580	-4.278077	-0.489439
39	6	0	0.405051	-3.909099	-1.703077
40	1	0	-0.076617	-3.836902	-2.682248
41	1	0	0.340004	-4.948633	-1.364339
42	1	0	1.457349	-3.641958	-1.818314

Zero-point correction=	0.369663
(Hartree/Particle)	
Thermal correction to Energy=	0.388713
Thermal correction to Enthalpy=	0.389657
Thermal correction to Gibbs Free Energy=	0.324704
Sum of electronic and zero-point Energies=	-821.818924
Sum of electronic and thermal Energies=	-821.799874
Sum of electronic and thermal Enthalpies=	-821.798930
Sum of electronic and thermal Free Energies=	-821.863884

IV

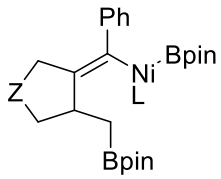


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.551399	-1.348636	-1.199426
2	6	0	-1.080289	-1.228341	-0.824220
3	6	0	-0.417406	-2.218321	-1.797340
4	6	0	-2.603051	-2.285069	-2.388982
5	1	0	-0.963981	-1.596949	0.197695
6	1	0	0.024938	-1.666542	-2.645350
7	1	0	0.361099	-2.817059	-1.321583
8	1	0	-3.478199	-2.935982	-2.422564
9	1	0	-2.575502	-1.695264	-3.323692
10	8	0	-1.442679	-3.085849	-2.269975
11	6	0	-3.592591	-0.732632	-0.611216
12	6	0	-0.471665	0.170393	-0.944155
13	1	0	-1.011116	0.871463	-0.296281
14	1	0	-0.635743	0.504793	-1.989932
15	28	0	1.425909	0.571455	-0.826915
16	5	0	-3.371196	0.231768	0.591977
17	8	0	-4.179221	1.319000	0.841358
18	8	0	-2.364531	0.105135	1.516855
19	6	0	-3.501967	2.140275	1.814672
20	6	0	-2.550255	1.117076	2.526247
21	6	0	-2.747149	3.213633	1.030248
22	1	0	-2.238210	3.916614	1.696624
23	1	0	-3.463726	3.768314	0.417271
24	1	0	-2.003553	2.761354	0.365654
25	6	0	-4.535020	2.786812	2.724182
26	1	0	-4.042294	3.357223	3.518891
27	1	0	-5.187358	2.039478	3.179845
28	1	0	-5.155471	3.474421	2.142126
29	6	0	-1.189160	1.679679	2.905082
30	1	0	-1.300141	2.502438	3.620574
31	1	0	-0.579298	0.895915	3.360367
32	6	0	-3.199738	0.428579	3.724132
33	1	0	-3.334829	1.120068	4.561277
34	1	0	-2.552411	-0.391312	4.049668
35	1	0	-4.173160	0.007741	3.453126
36	1	0	-0.648145	2.036539	2.025420
37	5	0	1.479801	-0.699631	0.632567
38	8	0	1.467399	-0.236217	1.956926
39	8	0	1.610836	-2.087206	0.637460
40	6	0	1.893842	-1.308995	2.814881
41	6	0	1.483017	-2.562966	1.991045
42	6	0	3.409275	-1.179458	2.976618
43	1	0	3.812906	-1.932624	3.661129
44	1	0	3.637820	-0.186581	3.375486
45	1	0	3.903021	-1.283579	2.004711
46	6	0	1.218964	-1.184744	4.172850
47	1	0	1.499967	-2.023974	4.819381
48	1	0	0.130660	-1.166496	4.082276
49	1	0	1.539501	-0.257593	4.658457
50	6	0	2.384631	-3.773965	2.170490

51	1	0	2.362725	-4.125161	3.208437
52	1	0	2.036202	-4.586075	1.524290
53	6	0	0.022892	-2.953258	2.221720
54	1	0	-0.108891	-3.441007	3.193477
55	1	0	-0.286914	-3.651129	1.437240
56	1	0	-0.630305	-2.075019	2.180703
57	1	0	3.415672	-3.540217	1.896774
58	1	0	5.268447	-4.187053	-0.054603
59	6	0	4.712795	-3.422704	-0.589086
60	7	0	3.279698	-1.450711	-1.952719
61	6	0	4.965661	-2.074474	-0.356303
62	6	0	3.734894	-3.768188	-1.511434
63	6	0	3.053625	-2.743935	-2.168559
64	6	0	4.214896	-1.125852	-1.051531
65	1	0	5.713788	-1.763356	0.366340
66	1	0	3.501085	-4.804887	-1.726931
67	1	0	2.291323	-2.976365	-2.907970
68	6	0	4.454666	0.330185	-0.856520
69	6	0	4.836835	3.043120	-0.742377
70	6	0	5.750464	0.830201	-0.713252
71	7	0	3.388136	1.141932	-0.887567
72	6	0	3.570793	2.473710	-0.873107
73	6	0	5.938171	2.203693	-0.637715
74	1	0	6.594343	0.149873	-0.701953
75	1	0	6.935424	2.618828	-0.537852
76	1	0	4.966357	4.118362	-0.747470
77	6	0	2.339807	3.286976	-1.061313
78	6	0	-0.006731	4.628812	-1.507340
79	6	0	2.291962	4.661392	-0.829373
80	7	0	1.262668	2.599910	-1.483126
81	6	0	0.122112	3.256397	-1.696767
82	6	0	1.100249	5.339810	-1.058490
83	1	0	3.159713	5.193691	-0.458163
84	1	0	-0.719594	2.649226	-2.018607
85	1	0	1.038567	6.408423	-0.881189
86	1	0	-0.955873	5.116813	-1.697289
87	6	0	-4.988162	-0.911074	-1.114641
88	6	0	-7.624336	-1.237320	-2.041541
89	6	0	-5.706472	0.173616	-1.632267
90	6	0	-5.623856	-2.157359	-1.052082
91	6	0	-6.927083	-2.321980	-1.514211
92	6	0	-7.009592	0.011826	-2.095769
93	1	0	-5.232540	1.150279	-1.666705
94	1	0	-5.086913	-3.001282	-0.626024
95	1	0	-7.400228	-3.297892	-1.455382
96	1	0	-7.546832	0.864937	-2.500207
97	1	0	-8.640514	-1.363111	-2.402607

Zero-point correction= 0.814721
(Hartree/Particle)
Thermal correction to Energy= 0.861483
Thermal correction to Enthalpy= 0.862428
Thermal correction to Gibbs Free Energy= 0.734786
Sum of electronic and zero-point Energies= -2272.340145
Sum of electronic and thermal Energies= -2272.293383
Sum of electronic and thermal Enthalpies= -2272.292439
Sum of electronic and thermal Free Energies= -2272.420081

v

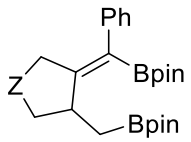


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.035659	-4.554592	-1.108394
2	6	0	1.561466	-4.324919	-0.137820
3	6	0	0.964982	-2.925040	-0.121924
4	6	0	-0.543504	-3.106929	-0.231779
5	6	0	-0.649826	-4.602642	-0.554792
6	8	0	0.465749	-5.205621	0.084806
7	1	0	2.303620	-4.490354	0.649052
8	1	0	-0.931341	-2.510693	-1.064718
9	1	0	-0.594440	-4.771412	-1.642807
10	1	0	-1.557517	-5.078809	-0.171070
11	6	0	1.590976	-1.751173	0.001078
12	6	0	-1.293013	-2.721072	1.055695
13	1	0	-0.757945	-1.881704	1.529137
14	1	0	-1.251345	-3.538899	1.787484
15	28	0	0.469482	-0.008410	0.143666
16	5	0	-2.751526	-2.201346	0.820513
17	5	0	-0.775277	1.593956	0.336383
18	8	0	-3.203032	-1.796077	-0.414695
19	8	0	-3.686515	-2.004085	1.807049
20	8	0	-0.454368	2.771291	1.004938
21	8	0	-1.945282	1.790212	-0.405292
22	6	0	-2.176069	3.207351	-0.503742
23	6	0	-1.508727	3.732345	0.799639
24	6	0	-1.453439	3.677297	-1.768250
25	1	0	-1.630934	4.738257	-1.971656
26	1	0	-1.816892	3.090289	-2.617928
27	1	0	-0.374185	3.510259	-1.677336
28	6	0	-0.901298	5.122638	0.686279
29	1	0	-1.669878	5.860579	0.429403
30	1	0	-0.118035	5.151796	-0.074254
31	1	0	-0.458983	5.410596	1.644719
32	6	0	-2.437698	3.662156	2.010769
33	1	0	-3.232423	4.412926	1.952969
34	1	0	-1.851124	3.846081	2.915588
35	1	0	-2.894270	2.670856	2.094218
36	6	0	-3.668422	3.474692	-0.613107
37	1	0	-3.873413	4.550700	-0.578499
38	1	0	-4.216504	2.986531	0.196805
39	1	0	-4.045462	3.087057	-1.564871
40	6	0	-4.590316	-1.418831	-0.280491
41	6	0	-4.717586	-1.154381	1.257140
42	6	0	-4.353505	0.279421	1.636471
43	1	0	-4.245016	0.338679	2.723657
44	1	0	-5.133235	0.983279	1.326060
45	1	0	-3.409584	0.579163	1.167893
46	6	0	-6.055672	-1.542719	1.864466
47	1	0	-6.256476	-2.608513	1.739276
48	1	0	-6.867207	-0.973240	1.398924
49	1	0	-6.050091	-1.317205	2.934719
50	6	0	-5.422249	-2.609067	-0.751305

51	1	0	-5.234999	-3.488995	-0.127603
52	1	0	-5.141840	-2.852542	-1.779876
53	1	0	-6.492394	-2.382401	-0.726853
54	6	0	-4.839545	-0.200065	-1.156102
55	1	0	-4.769540	-0.488738	-2.210229
56	1	0	-4.092894	0.574260	-0.959334
57	1	0	-5.841922	0.206865	-0.982239
58	7	0	1.483634	0.558879	1.843061
59	6	0	3.005432	1.345856	4.038444
60	6	0	2.661396	1.200238	1.665258
61	6	0	1.070166	0.313409	3.089661
62	6	0	1.797639	0.676706	4.215964
63	6	0	3.437366	1.614746	2.747681
64	1	0	0.115988	-0.196971	3.179594
65	1	0	1.416597	0.444075	5.203531
66	1	0	4.368031	2.143019	2.572128
67	1	0	3.598253	1.655894	4.892645
68	7	0	2.111255	1.220759	-0.612978
69	6	0	4.583208	1.746582	-1.578911
70	6	0	2.289805	1.183260	-1.921052
71	6	0	3.091931	1.411149	0.252952
72	6	0	4.382065	1.697789	-0.199541
73	6	0	3.543047	1.470315	-2.467309
74	1	0	5.213481	1.831134	0.483539
75	1	0	3.724959	1.441382	-3.536409
76	1	0	5.575729	1.952408	-1.966875
77	6	0	3.061190	-1.721643	0.083715
78	6	0	5.881841	-1.486634	0.220664
79	6	0	3.733269	-1.653392	1.318186
80	6	0	3.852790	-1.682560	-1.079399
81	6	0	5.237223	-1.567777	-1.013676
82	6	0	5.119405	-1.538210	1.386568
83	1	0	3.146531	-1.683567	2.234505
84	1	0	3.357083	-1.739983	-2.046530
85	1	0	5.818219	-1.535925	-1.932177
86	1	0	5.605459	-1.484743	2.357625
87	1	0	6.962556	-1.393038	0.272893
88	6	0	1.060247	0.754128	-2.651386
89	6	0	-1.277721	-0.012146	-3.858683
90	6	0	0.893926	0.977141	-4.016232
91	6	0	-0.288188	0.582138	-4.632242
92	6	0	-1.046283	-0.194316	-2.498123
93	1	0	1.676045	1.473471	-4.580330
94	1	0	-0.436343	0.749096	-5.694181
95	1	0	-1.803993	-0.629275	-1.851947
96	1	0	-2.221561	-0.327471	-4.289103
97	7	0	0.098228	0.159224	-1.904554

Zero-point correction= 0.814011
(Hartree/Particle)
Thermal correction to Energy= 0.860737
Thermal correction to Enthalpy= 0.861682
Thermal correction to Gibbs Free Energy= 0.735597
Sum of electronic and zero-point Energies= -2272.330596
Sum of electronic and thermal Energies= -2272.283870
Sum of electronic and thermal Enthalpies= -2272.282926
Sum of electronic and thermal Free Energies= -2272.409010

VI

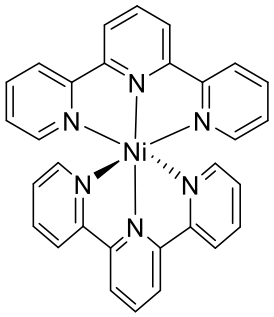


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.521959	-3.369959	-1.362641
2	6	0	2.003055	-3.128069	-0.420794
3	6	0	1.530927	-1.685490	-0.421069
4	6	0	0.023304	-1.738902	-0.629859
5	6	0	-0.160960	-3.198770	-1.059464
6	8	0	0.823247	-3.909204	-0.322300
7	1	0	2.669034	-3.372892	0.411997
8	1	0	-0.300736	-1.035674	-1.401322
9	1	0	0.013313	-3.319019	-2.139923
10	1	0	-1.140107	-3.615194	-0.806127
11	6	0	2.234330	-0.566959	-0.174197
12	6	0	-0.727615	-1.465701	0.690873
13	1	0	-0.611504	-2.326595	1.360048
14	5	0	-2.236314	-1.079646	0.494271
15	5	0	1.479006	0.807533	-0.212864
16	8	0	-3.262120	-1.446781	1.325412
17	8	0	-2.652604	-0.257192	-0.527012
18	8	0	0.750707	1.218942	-1.299738
19	8	0	1.461059	1.726931	0.808285
20	6	0	0.485731	2.739905	0.462952
21	6	0	0.399894	2.605565	-1.091157
22	6	0	-0.820841	2.358587	1.155966
23	1	0	-1.577849	3.139704	1.029631
24	1	0	-0.631714	2.224067	2.225000
25	1	0	-1.220758	1.425625	0.747286
26	6	0	-0.982065	2.851837	-1.676223
27	1	0	-1.334607	3.856992	-1.420306
28	1	0	-1.697974	2.112301	-1.309706
29	1	0	-0.935737	2.773378	-2.766339
30	6	0	1.452357	3.439752	-1.817044
31	1	0	1.222756	4.507907	-1.759613
32	1	0	1.473494	3.143457	-2.869125
33	1	0	2.447172	3.270982	-1.392521
34	6	0	0.978948	4.086812	0.965903
35	1	0	0.307298	4.886576	0.636517
36	1	0	1.986997	4.302291	0.606054
37	1	0	0.996678	4.084001	2.059493
38	6	0	-4.402919	-0.623458	0.987159
39	6	0	-4.097494	-0.225503	-0.493779
40	6	0	-4.585204	-1.264285	-1.500942
41	1	0	-4.168585	-1.026390	-2.483464
42	1	0	-5.676566	-1.266730	-1.575977
43	1	0	-4.250849	-2.268257	-1.219890
44	6	0	-4.567518	1.164406	-0.890563
45	1	0	-4.094110	1.933807	-0.275422
46	1	0	-5.654425	1.248025	-0.784533
47	1	0	-4.309647	1.353897	-1.936713
48	6	0	-4.381713	0.570404	1.939211
49	1	0	-3.469263	1.161476	1.805477
50	1	0	-4.402732	0.201698	2.968137
51	1	0	-5.246834	1.221421	1.782845

52	6	0	-5.673718	-1.433860	1.181102
53	1	0	-5.798730	-1.670272	2.241496
54	1	0	-5.638328	-2.370984	0.622283
55	1	0	-6.547018	-0.860145	0.853190
56	6	0	3.684975	-0.583363	0.153804
57	6	0	6.421079	-0.595901	0.820036
58	6	0	4.185242	0.253557	1.163240
59	6	0	4.589979	-1.407099	-0.528908
60	6	0	5.942459	-1.416360	-0.198433
61	6	0	5.535893	0.240695	1.496822
62	1	0	3.501535	0.909786	1.692952
63	1	0	4.237035	-2.025969	-1.348074
64	1	0	6.623942	-2.060764	-0.745831
65	1	0	5.898881	0.889408	2.288537
66	1	0	7.475402	-0.602643	1.078660
67	1	0	-0.251945	-0.623117	1.215906

Zero-point correction= 0.583345
(Hartree/Particle)
Thermal correction to Energy= 0.614084
Thermal correction to Enthalpy= 0.615028
Thermal correction to Gibbs Free Energy= 0.521730
Sum of electronic and zero-point Energies= -1361.111151
Sum of electronic and thermal Energies= -1361.080411
Sum of electronic and thermal Enthalpies= -1361.079467
Sum of electronic and thermal Free Energies= -1361.172765

- ***Ni(tpy)₂***



B3LYP / Gas

	Singlet	Triplet	Quintet	Dif(s-t)	Dif(t-q)
E+ZPE	-1653.811529	-1653.861149	-1653.862269	31,138	0,703
G	-1653.873602	-1653.923901	-1653.924166	31,564	0,166

M062X / diisopropylether

	Singlet	Triplet	Quintet	Dif(s-t)	Dif(t-q)
E+ZPE	-1653.218724	-1653.255040	-1653.285408	22,789	19,057
G	-1653.278160	-1653.318266	-1653.347544	25,167	18,373

- ***COORDINATES – B3LYP***

(tpy)₂Ni – Singlet (*TPY2-Ni_B3L_s*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.956973	-1.906915	-4.652503
2	6	0	2.448400	-1.583153	-3.748896
3	7	0	1.102411	-0.740368	-1.428350
4	6	0	2.887781	-0.471053	-3.054920
5	6	0	1.310329	-2.272429	-3.275813
6	6	0	0.672589	-1.802362	-2.141861
7	6	0	2.219565	-0.062115	-1.885214
8	1	0	3.736189	0.105039	-3.412196
9	1	0	0.935822	-3.157181	-3.780812
10	1	0	-0.218488	-2.286544	-1.755305
11	6	0	2.559070	1.080851	-1.075813
12	6	0	2.951567	3.070903	0.820406
13	6	0	3.779789	1.749944	-1.029112
14	7	0	1.511980	1.476830	-0.265081
15	6	0	1.746468	2.381977	0.749292
16	6	0	3.971440	2.779434	-0.099628

17	1	0	4.589099	1.448570	-1.687869
18	1	0	4.924576	3.295437	-0.041540
19	1	0	3.116416	3.801498	1.606753
20	6	0	0.654822	2.441416	1.695986
21	6	0	-1.495802	2.273127	3.423472
22	6	0	0.454103	3.449567	2.656079
23	7	0	-0.219495	1.378282	1.589230
24	6	0	-1.261379	1.324552	2.442034
25	6	0	-0.615289	3.368142	3.529749
26	1	0	1.138840	4.291159	2.696307
27	1	0	-1.920125	0.470379	2.326301
28	1	0	-0.777103	4.139684	4.277052
29	1	0	-2.340253	2.158650	4.095313
30	28	0	0.109636	0.251598	0.000503
31	1	0	-4.858286	1.703863	-3.583436
32	6	0	-3.993559	1.592815	-2.934360
33	7	0	-1.765518	1.277364	-1.290488
34	6	0	-3.946361	0.560197	-2.007677
35	6	0	-2.905614	2.468728	-3.039503
36	6	0	-1.811950	2.249702	-2.202990
37	6	0	-2.812089	0.431374	-1.176845
38	1	0	-4.756568	-0.159498	-1.953133
39	1	0	-2.905614	3.291852	-3.747257
40	1	0	-0.930385	2.886869	-2.251312
41	6	0	-2.692085	-0.639928	-0.177690
42	6	0	-2.421646	-2.830738	1.476910
43	6	0	-3.836580	-1.255244	0.361584
44	7	0	-1.424084	-1.056389	0.171732
45	6	0	-1.315400	-2.154080	0.973007
46	6	0	-3.712797	-2.353453	1.194350
47	1	0	-4.816664	-0.852292	0.128499
48	1	0	-4.588472	-2.828873	1.625908
49	1	0	-2.271649	-3.700473	2.107481
50	6	0	0.046690	-2.672838	1.310080
51	6	0	2.535105	-3.606448	1.988407
52	6	0	0.358815	-4.018849	1.067271
53	7	0	0.919623	-1.821764	1.871252
54	6	0	2.128636	-2.285767	2.198382
55	6	0	1.625473	-4.489924	1.412158
56	1	0	-0.373853	-4.673375	0.605217
57	1	0	2.804261	-1.565180	2.655427
58	1	0	1.896385	-5.525750	1.225708
59	1	0	3.534116	-3.925432	2.270181

Zero-point correction=	0.454397
(Hartree/Particle)	
Thermal correction to Energy=	0.483764
Thermal correction to Enthalpy=	0.484708
Thermal correction to Gibbs Free Energy=	0.392324
Sum of electronic and zero-point Energies=	-1653.811529
Sum of electronic and thermal Energies=	-1653.782162
Sum of electronic and thermal Enthalpies=	-1653.781218
Sum of electronic and thermal Free Energies=	-1653.873602

TPY2Ni – Triplet (*TPY2-Ni_B3L_t*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.771788	-0.132424	5.781528
2	6	0	-1.412673	-0.109718	4.756220
3	7	0	-0.495117	-0.050892	2.125069
4	6	0	-2.312862	-0.084695	3.705153
5	6	0	-0.032635	-0.105448	4.481865
6	6	0	0.365257	-0.075686	3.152156
7	6	0	-1.840584	-0.054899	2.376191
8	1	0	-3.379662	-0.087806	3.902821
9	1	0	0.705543	-0.124576	5.276746
10	1	0	1.417167	-0.071272	2.877318
11	6	0	-2.695748	-0.026653	1.193683
12	6	0	-4.088657	0.028355	-1.209812
13	6	0	-4.088336	-0.026460	1.210865
14	7	0	-2.014311	0.000516	0.000194
15	6	0	-2.696060	0.027967	-1.193080
16	6	0	-4.796613	0.001108	0.000628
17	1	0	-4.629319	-0.047953	2.151414
18	1	0	-5.881919	0.001346	0.000815
19	1	0	-4.629880	0.050090	-2.150228
20	6	0	-1.841275	0.055956	-2.375886
21	6	0	-0.034067	0.106007	-4.482206
22	6	0	-2.314029	0.086044	-3.704671
23	7	0	-0.495777	0.051422	-2.125248
24	6	0	0.364247	0.075976	-3.152599
25	6	0	-1.414186	0.110825	-4.756062
26	1	0	-3.380897	0.089583	-3.901960
27	1	0	1.416251	0.071043	-2.878121
28	1	0	-1.773654	0.133730	-5.781246
29	1	0	0.703825	0.124911	-5.277360
30	28	0	-0.003003	-0.000035	0.000295
31	1	0	1.778644	5.781367	0.133256
32	6	0	1.417556	4.756751	0.110361
33	7	0	0.495519	2.127199	0.051052
34	6	0	2.315897	3.703938	0.085288
35	6	0	0.037039	4.484928	0.105860
36	6	0	-0.362767	3.155498	0.075855
37	6	0	1.841497	2.375853	0.055233
38	1	0	3.382998	3.899929	0.088596
39	1	0	-0.699894	5.280937	0.124975
40	1	0	-1.415254	2.882704	0.071197
41	6	0	2.696082	1.191940	0.026868
42	6	0	4.087922	-1.212069	-0.028183
43	6	0	4.088804	1.209376	0.026661
44	7	0	2.015415	-0.000643	-0.000324
45	6	0	2.695281	-1.193644	-0.027754
46	6	0	4.796239	-0.001550	-0.000964
47	1	0	4.630498	2.149491	0.048127
48	1	0	5.881574	-0.001946	-0.001255
49	1	0	4.628977	-2.152538	-0.049968
50	6	0	1.839822	-2.377005	-0.055667
51	6	0	0.033861	-4.484778	-0.105427
52	6	0	2.313272	-3.705407	-0.085423

53	7	0	0.494059	-2.127379	-0.051365
54	6	0	-0.365001	-3.155055	-0.075740
55	6	0	1.414151	-4.757588	-0.110053
56	1	0	3.380227	-3.902195	-0.088778
57	1	0	-1.417286	-2.881499	-0.071048
58	1	0	1.774500	-5.782470	-0.132699
59	1	0	-0.703658	-5.280252	-0.124217

Zero-point correction= 0.451365
(Hartree/Particle)
Thermal correction to Energy= 0.481205
Thermal correction to Enthalpy= 0.482149
Thermal correction to Gibbs Free Energy= 0.388613
Sum of electronic and zero-point Energies= -1653.861149
Sum of electronic and thermal Energies= -1653.831309
Sum of electronic and thermal Enthalpies= -1653.830365
Sum of electronic and thermal Free Energies= -1653.923901

TPY2Ni – Quintet (*TPY2-Ni_B3L_q*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.763751	4.596086	3.510844
2	6	0	1.405891	3.780686	2.888126
3	7	0	0.491857	1.688226	1.290110
4	6	0	2.307413	2.946223	2.250433
5	6	0	0.026168	3.560997	2.720885
6	6	0	-0.369969	2.503587	1.913258
7	6	0	1.837054	1.889269	1.443257
8	1	0	3.373955	3.104640	2.371251
9	1	0	-0.713054	4.191915	3.203164
10	1	0	-1.421444	2.283749	1.745672
11	6	0	2.693379	0.950036	0.725740
12	6	0	4.087821	-0.959921	-0.732946
13	6	0	4.086004	0.964486	0.736703
14	7	0	2.012782	0.001061	0.000905
15	6	0	2.695168	-0.947108	-0.723314
16	6	0	4.794901	0.002693	0.002217
17	1	0	4.626408	1.712443	1.307909
18	1	0	5.880219	0.003325	0.002730
19	1	0	4.629644	-1.707236	-1.303651
20	6	0	1.840698	-1.887352	-1.441732
21	6	0	0.033221	-3.561230	-2.721390
22	6	0	2.313204	-2.943777	-2.248349
23	7	0	0.495093	-1.687888	-1.290122
24	6	0	-0.365069	-2.504264	-1.914245
25	6	0	1.413389	-3.779313	-2.887047
26	1	0	3.380068	-3.100947	-2.367940
27	1	0	-1.416989	-2.285630	-1.747887
28	1	0	1.772914	-4.594312	-3.509331
29	1	0	-0.704714	-4.193020	-3.204498
30	28	0	0.000002	-0.000048	-0.000043
31	1	0	-1.768452	-3.511053	4.594455
32	6	0	-1.409742	-2.888415	3.779367

33	7	0	-0.493530	-1.290587	1.687700
34	6	0	-2.310394	-2.250526	2.944116
35	6	0	-0.029789	-2.721472	3.560873
36	6	0	0.367444	-1.913935	2.503810
37	6	0	-1.838939	-1.443443	1.887578
38	1	0	-3.377100	-2.371113	3.101599
39	1	0	0.708787	-3.203911	4.192424
40	1	0	1.419153	-1.746605	2.284888
41	6	0	-2.694294	-0.725775	0.947596
42	6	0	-4.086901	0.733095	-0.963609
43	6	0	-4.086946	-0.736610	0.960772
44	7	0	-2.012814	-0.000949	-0.000756
45	6	0	-2.694265	0.723325	-0.949519
46	6	0	-4.794901	-0.002039	-0.001637
47	1	0	-4.628094	-1.307792	1.708209
48	1	0	-5.880220	-0.002467	-0.001989
49	1	0	-4.628013	1.303850	-1.711397
50	6	0	-1.838830	1.441634	-1.888969
51	6	0	-0.029564	2.720915	-3.561159
52	6	0	-2.310209	2.248409	-2.945761
53	7	0	-0.493448	1.289661	-1.688301
54	6	0	0.367589	1.913607	-2.503885
55	6	0	-1.409493	2.886935	-3.780464
56	1	0	-3.376903	2.368272	-3.103875
57	1	0	1.419278	1.746962	-2.284350
58	1	0	-1.768143	3.509353	-4.595746
59	1	0	0.709058	3.203864	-4.192266

Zero-point correction= 0.452199
(Hartree/Particle)
Thermal correction to Energy= 0.481605
Thermal correction to Enthalpy= 0.482549
Thermal correction to Gibbs Free Energy= 0.390302
Sum of electronic and zero-point Energies= -1653.862269
Sum of electronic and thermal Energies= -1653.832863
Sum of electronic and thermal Enthalpies= -1653.831919
Sum of electronic and thermal Free Energies= -1653.924166

- ***COORDINATES – M062X / DIE***

TPY2Ni – Singlet (*TPY2-Ni_M06_DIE_s*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.555835	2.066345	2.909289
2	6	0	3.662945	1.670355	2.434459
3	7	0	1.361030	0.680090	1.200370
4	6	0	3.587835	0.344104	2.110079
5	6	0	2.554504	2.523955	2.170972
6	6	0	1.447211	1.971065	1.574352
7	6	0	2.421477	-0.176598	1.479649
8	1	0	4.409236	-0.328938	2.336079
9	1	0	2.571802	3.575649	2.430244
10	1	0	0.571772	2.579788	1.355393

11	6	0	2.170521	-1.517531	1.135950
12	6	0	1.465864	-3.931059	-0.056067
13	6	0	3.089058	-2.568945	1.099142
14	7	0	0.813534	-1.770318	0.809059
15	6	0	0.570649	-2.891093	0.008845
16	6	0	2.732226	-3.804193	0.573366
17	1	0	4.110190	-2.395349	1.430791
18	1	0	3.453415	-4.611523	0.518704
19	1	0	1.232620	-4.814445	-0.643650
20	6	0	-0.667226	-2.805234	-0.717331
21	6	0	-3.050426	-2.336447	-2.043997
22	6	0	-1.351679	-3.878834	-1.324401
23	7	0	-1.197038	-1.540980	-0.748524
24	6	0	-2.351541	-1.334917	-1.403538
25	6	0	-2.531769	-3.646785	-1.992768
26	1	0	-0.940041	-4.879800	-1.250682
27	1	0	-2.714056	-0.310577	-1.412432
28	1	0	-3.060351	-4.465350	-2.471076
29	1	0	-3.971017	-2.110311	-2.568369
30	28	0	-0.100479	-0.240062	0.276570
31	1	0	-6.077477	0.497405	1.628131
32	6	0	-4.992402	0.485616	1.624887
33	7	0	-2.211214	0.442714	1.593026
34	6	0	-4.285545	1.287147	0.734995
35	6	0	-4.287923	-0.339427	2.494936
36	6	0	-2.895686	-0.327445	2.436060
37	6	0	-2.890217	1.232639	0.756324
38	1	0	-4.806889	1.915477	0.020865
39	1	0	-4.799693	-0.984368	3.200205
40	1	0	-2.299643	-0.961129	3.087066
41	6	0	-2.064257	2.036214	-0.188432
42	6	0	-0.461693	3.449390	-1.898835
43	6	0	-2.505540	3.269858	-0.667762
44	7	0	-0.874292	1.521601	-0.541308
45	6	0	-0.075362	2.215537	-1.373386
46	6	0	-1.693509	3.980470	-1.541508
47	1	0	-3.455729	3.673193	-0.337588
48	1	0	-2.014614	4.940509	-1.931893
49	1	0	0.197927	3.969629	-2.584303
50	6	0	1.272320	1.646515	-1.668057
51	6	0	3.730888	0.503584	-1.927009
52	6	0	2.395081	2.470443	-1.636505
53	7	0	1.338201	0.323705	-1.862333
54	6	0	2.543543	-0.231636	-1.974981
55	6	0	3.651746	1.879403	-1.770631
56	1	0	2.294326	3.536346	-1.460975
57	1	0	2.560540	-1.311078	-2.105714
58	1	0	4.549990	2.487001	-1.730610
59	1	0	4.687164	-0.001341	-2.008313

Zero-point correction= 0.460270
(Hartree/Particle)
Thermal correction to Energy= 0.489007
Thermal correction to Enthalpy= 0.489951
Thermal correction to Gibbs Free Energy= 0.400834
Sum of electronic and zero-point Energies= -1653.218724
Sum of electronic and thermal Energies= -1653.189987

```
 Sum of electronic and thermal Enthalpies=           -1653.189043
 Sum of electronic and thermal Free Energies=        -1653.278160
```

TPY2Ni – Triplet (*TPY2-Ni_M06_DIE_t*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.501843	-1.732421	2.043594
2	6	0	4.497616	-1.394788	1.806171
3	7	0	1.929304	-0.530885	1.171432
4	6	0	3.574493	-2.280842	1.287627
5	6	0	4.126451	-0.058195	2.015343
6	6	0	2.831626	0.310574	1.675368
7	6	0	2.274996	-1.830697	0.973653
8	1	0	3.859206	-3.310856	1.105403
9	1	0	4.817979	0.669082	2.424199
10	1	0	2.491772	1.336979	1.802897
11	6	0	1.246455	-2.694399	0.399755
12	6	0	-0.757695	-4.176674	-0.802265
13	6	0	1.404478	-4.086792	0.243584
14	7	0	0.098468	-2.084191	-0.001747
15	6	0	-0.857955	-2.803341	-0.602320
16	6	0	0.402905	-4.825182	-0.352615
17	1	0	2.302667	-4.580878	0.595563
18	1	0	0.517575	-5.896766	-0.481791
19	1	0	-1.544163	-4.717468	-1.315845
20	6	0	-2.056125	-2.042292	-1.058526
21	6	0	-4.203813	-0.519687	-1.792786
22	6	0	-3.337921	-2.591649	-0.962439
23	7	0	-1.834811	-0.805083	-1.519382
24	6	0	-2.888101	-0.068288	-1.870843
25	6	0	-4.427983	-1.814474	-1.336235
26	1	0	-3.474480	-3.592730	-0.566903
27	1	0	-2.666132	0.936845	-2.223506
28	1	0	-5.436365	-2.208370	-1.255449
29	1	0	-5.024070	0.127967	-2.081971
30	28	0	-0.000127	-0.000067	0.334101
31	1	0	-5.501845	1.733328	2.043275
32	6	0	-4.497654	1.395556	1.805892
33	7	0	-1.929445	0.531311	1.171260
34	6	0	-3.574416	2.281473	1.287324
35	6	0	-4.126665	0.058918	2.015134
36	6	0	-2.831875	-0.310021	1.675213
37	6	0	-2.274962	1.831153	0.973399
38	1	0	-3.858994	3.311514	1.105044
39	1	0	-4.818296	-0.668248	2.424014
40	1	0	-2.492142	-1.336461	1.802790
41	6	0	-1.246291	2.694659	0.399470
42	6	0	0.758095	4.176535	-0.802662
43	6	0	-1.404078	4.087080	0.243239
44	7	0	-0.098415	2.084242	-0.002027
45	6	0	0.858107	2.803188	-0.602659
46	6	0	-0.402388	4.825263	-0.353014
47	1	0	-2.302172	4.581339	0.595223
48	1	0	-0.516868	5.896862	-0.482227

49	1	0	1.544646	4.717172	-1.316280
50	6	0	2.056148	2.041896	-1.058821
51	6	0	4.203573	0.518858	-1.792954
52	6	0	3.338035	2.591051	-0.962823
53	7	0	1.834620	0.804688	-1.519573
54	6	0	2.887781	0.067682	-1.870968
55	6	0	4.427965	1.813652	-1.336541
56	1	0	3.474769	3.592150	-0.567392
57	1	0	2.665640	-0.937449	-2.223530
58	1	0	5.436414	2.207389	-1.255804
59	1	0	5.023715	-0.128971	-2.082073

Zero-point correction= 0.461028
(Hartree/Particle)
Thermal correction to Energy= 0.490639
Thermal correction to Enthalpy= 0.491583
Thermal correction to Gibbs Free Energy= 0.397801
Sum of electronic and zero-point Energies= -1653.255040
Sum of electronic and thermal Energies= -1653.225429
Sum of electronic and thermal Enthalpies= -1653.224485
Sum of electronic and thermal Free Energies= -1653.318266

TPY2Ni – Quintet (*TPY2-Ni_M06_DIE_q*)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.858435	3.583800	3.957327
2	6	0	2.307434	2.949964	3.268641
3	7	0	0.887240	1.327665	1.509348
4	6	0	2.976179	2.024146	2.506675
5	6	0	0.903754	3.073057	3.155130
6	6	0	0.259987	2.235803	2.262247
7	6	0	2.255202	1.192724	1.607118
8	1	0	4.053115	1.922722	2.591488
9	1	0	0.344229	3.790704	3.742507
10	1	0	-0.820067	2.278562	2.127864
11	6	0	2.847605	0.195803	0.771704
12	6	0	3.719048	-1.793193	-0.996552
13	6	0	4.231106	-0.113434	0.677943
14	7	0	1.963548	-0.511264	-0.011688
15	6	0	2.387012	-1.459990	-0.864133
16	6	0	4.656887	-1.089490	-0.187568
17	1	0	4.951408	0.423374	1.286614
18	1	0	5.713351	-1.325966	-0.262227
19	1	0	4.054285	-2.553436	-1.690816
20	6	0	1.283841	-2.093966	-1.642922
21	6	0	-0.888932	-3.130456	-2.978433
22	6	0	1.471716	-3.153804	-2.531932
23	7	0	0.058876	-1.577045	-1.433280
24	6	0	-0.995112	-2.079031	-2.075864
25	6	0	0.373457	-3.673011	-3.205861
26	1	0	2.459157	-3.571366	-2.689032
27	1	0	-1.950787	-1.612531	-1.846308
28	1	0	0.501726	-4.496575	-3.900922

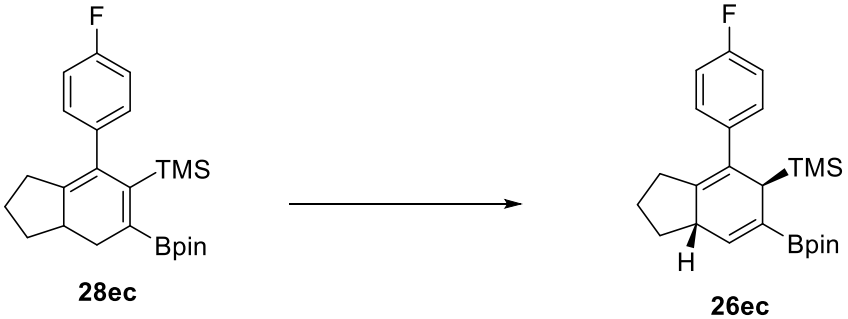
29	1	0	-1.769718	-3.511455	-3.481950
30	28	0	-0.000075	-0.000198	0.088567
31	1	0	-2.862820	-3.581559	3.956311
32	6	0	-2.311128	-2.948248	3.267701
33	7	0	-0.889096	-1.327264	1.508689
34	6	0	-2.978993	-2.022491	2.504905
35	6	0	-0.907412	-3.071978	3.155159
36	6	0	-0.262707	-2.235345	2.262379
37	6	0	-2.257095	-1.191768	1.605423
38	1	0	-4.055939	-1.920553	2.589001
39	1	0	-0.348554	-3.789599	3.743204
40	1	0	0.817430	-2.278543	2.128790
41	6	0	-2.848467	-0.195069	0.769010
42	6	0	-3.717655	1.794248	-0.999971
43	6	0	-4.231688	0.115146	0.674580
44	7	0	-1.963587	0.510888	-0.014454
45	6	0	-2.385919	1.459918	-0.867084
46	6	0	-4.656351	1.091347	-0.191315
47	1	0	-4.952651	-0.421006	1.283039
48	1	0	-5.712604	1.328597	-0.266478
49	1	0	-4.052035	2.554953	-1.694146
50	6	0	-1.281928	2.092977	-1.645469
51	6	0	0.892165	3.128020	-2.979911
52	6	0	-1.468941	3.151731	-2.535950
53	7	0	-0.057187	1.576322	-1.433984
54	6	0	0.997449	2.077615	-2.076030
55	6	0	-0.370002	3.670227	-3.209333
56	1	0	-2.456268	3.568926	-2.694709
57	1	0	1.952896	1.611334	-1.845065
58	1	0	-0.497611	4.492873	-3.905589
59	1	0	1.773483	3.508448	-3.482931

Zero-point correction= 0.459189
(Hartree/Particle)
Thermal correction to Energy= 0.488206
Thermal correction to Enthalpy= 0.489150
Thermal correction to Gibbs Free Energy= 0.397052
Sum of electronic and zero-point Energies= -1653.285408
Sum of electronic and thermal Energies= -1653.256391
Sum of electronic and thermal Enthalpies= -1653.255447
Sum of electronic and thermal Free Energies= -1653.347544

Computational results: Chapter 5

- **Thermodynamic stability of compounds 26 and 28**

M06

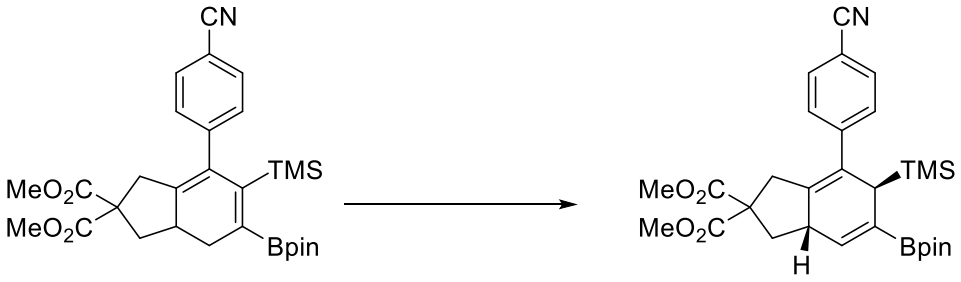


28ec **26ec**

E+ZPE = -1498.372018
G = -1498.431007

Δ(E+ZPE) = -6,130 Kcal/mol
ΔG = -6,435 Kcal/mol

-1498.381787
-1498.441261

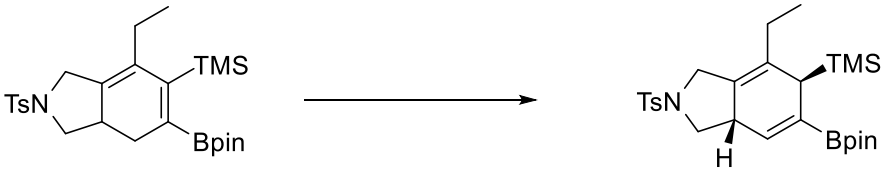


28cf **26cf**

E+ZPE = -1946.761533
G = -1946.833667

Δ(E+ZPE) = -5.239 Kcal/mol
ΔG = -5,372 Kcal/mol

-1946.769881
-1946.842228



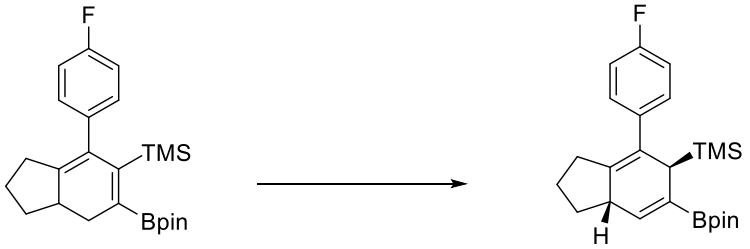
28bo **26bo**

E+ZPE = -2081.431853
G = -2081.498825

Δ(E+ZPE) = -7.362 Kcal/mol
ΔG = -7.918 Kcal/mol

-2081.443585
-2081.511443

B3LYP

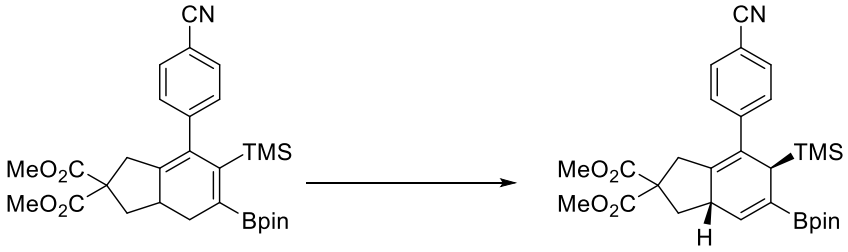


28ec **26ec**

E+ZPE = -1499.245087
G = -1499.305991

Δ(E+ZPE) = -3,909 Kcal/mol
ΔG = -4,511 Kcal/mol

-1499.251317
-1499.313179



28cf **26cf**

E+ZPE = -1947.886036
G = -1947.960780

Δ(E+ZPE) = -5.072 Kcal/mol
ΔG = -5,618 Kcal/mol

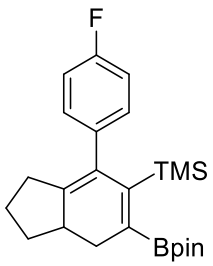
-1947.894119
-1947.969733

CARTESIAN COORDINATES – M06

- ***Computational methods***

Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the M06 hybrid functional[2] that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, N, O, F, S, B and Si. Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Gibbs free energy has been used throughout the schemes. Solvent effects were considered by performing optimizations in Toluene using the polarized continuum model (PCM).

28ec



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.672224	0.773368	-0.179642
2	6	0	-0.768679	0.762717	-0.009287
3	6	0	0.430439	2.905635	-0.420704
4	6	0	-0.666526	2.231041	0.376211
5	6	0	1.710104	2.117047	-0.271425
6	6	0	0.365280	0.073086	-0.298389
7	1	0	0.136488	2.923574	-1.489493
8	1	0	-0.431569	2.308233	1.455898
9	1	0	-1.630385	2.746078	0.233403
10	14	0	0.203455	-1.714220	-0.930637
11	6	0	1.804382	-2.483525	-1.558651
12	1	0	1.548547	-3.410367	-2.092920
13	1	0	2.512280	-2.735470	-0.759884
14	1	0	2.319605	-1.824226	-2.269963
15	6	0	-0.949198	-1.694534	-2.427118
16	1	0	-1.864164	-1.109995	-2.274972
17	1	0	-1.236670	-2.721290	-2.698115
18	1	0	-0.420522	-1.261214	-3.287727
19	6	0	-0.507839	-2.820908	0.423450

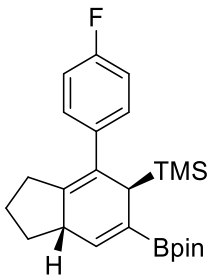
[1] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. 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.

[2] Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, *120*: 215–241.

20	1	0	-0.808319	-3.792467	0.005504
21	1	0	-1.381949	-2.371133	0.914065
22	1	0	0.244893	-3.012505	1.200795
23	5	0	-2.230934	0.231581	0.096601
24	8	0	-2.734435	-0.275606	1.268490
25	8	0	-3.188317	0.363391	-0.877007
26	6	0	-4.174070	-0.270607	1.147898
27	6	0	-4.378027	-0.304643	-0.395562
28	6	0	-5.595541	0.444197	-0.895565
29	1	0	-5.656305	0.363949	-1.988010
30	1	0	-5.554688	1.507417	-0.637052
31	1	0	-6.514988	0.014819	-0.473684
32	6	0	-4.363068	-1.713371	-0.971141
33	1	0	-4.304997	-1.650253	-2.065056
34	1	0	-5.274688	-2.265127	-0.707719
35	1	0	-3.494714	-2.288281	-0.620664
36	6	0	-4.657671	1.023491	1.786621
37	1	0	-5.753170	1.091270	1.789601
38	1	0	-4.256066	1.903179	1.265079
39	1	0	-4.307234	1.058827	2.825354
40	6	0	-4.732668	-1.462925	1.895642
41	1	0	-5.820334	-1.534831	1.756495
42	1	0	-4.537011	-1.349664	2.969170
43	1	0	-4.273628	-2.401820	1.566261
44	6	0	2.874465	3.064519	-0.117789
45	1	0	3.735786	2.818888	-0.751502
46	1	0	3.243125	3.032464	0.921642
47	6	0	0.823020	4.315794	0.022398
48	1	0	0.164247	5.095966	-0.379215
49	1	0	0.773492	4.374060	1.122720
50	6	0	2.275367	4.440574	-0.434738
51	1	0	2.815741	5.266402	0.043294
52	1	0	2.304453	4.615566	-1.521101
53	6	0	2.883834	-0.017599	0.143183
54	6	0	5.121255	-1.530366	0.807246
55	6	0	2.888799	-0.833291	1.281591
56	6	0	4.035630	0.019659	-0.648785
57	6	0	5.158556	-0.733755	-0.326155
58	6	0	4.001878	-1.592970	1.622499
59	1	0	2.000362	-0.864481	1.913831
60	1	0	4.039788	0.627644	-1.553262
61	1	0	6.054758	-0.720577	-0.942449
62	1	0	4.017019	-2.225256	2.507403
63	9	0	6.198605	-2.260700	1.125066

Zero-point correction= 0.533597
(Hartree/Particle)
Thermal correction to Energy= 0.563793
Thermal correction to Enthalpy= 0.564738
Thermal correction to Gibbs Free Energy= 0.474608
Sum of electronic and zero-point Energies= -1498.372018
Sum of electronic and thermal Energies= -1498.341821
Sum of electronic and thermal Enthalpies= -1498.340877
Sum of electronic and thermal Free Energies= -1498.431007

26ec

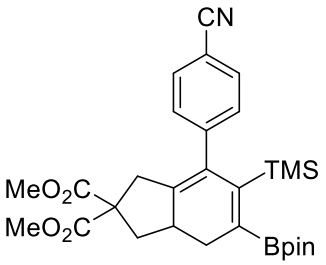


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.590731	0.620058	-0.141773
2	6	0	0.915138	0.852216	0.027023
3	6	0	-0.539790	2.869065	0.197953
4	6	0	-1.705320	1.958452	-0.109843
5	1	0	-0.645619	3.259003	1.232742
6	14	0	-0.348160	-0.725006	1.995391
7	6	0	-1.005288	0.613117	3.145189
8	1	0	-1.031535	0.248256	4.180987
9	1	0	-2.021570	0.924965	2.870582
10	1	0	-0.360718	1.502626	3.123353
11	6	0	1.380459	-1.209437	2.571456
12	1	0	1.830769	-1.958300	1.906598
13	1	0	1.339617	-1.630294	3.585453
14	1	0	2.044882	-0.333379	2.598920
15	6	0	-1.457255	-2.247140	2.047356
16	1	0	-1.446202	-2.700074	3.048385
17	1	0	-1.106108	-3.005909	1.334050
18	1	0	-2.499173	-2.010842	1.792393
19	5	0	2.308728	0.234511	-0.242279
20	8	0	2.495349	-1.088968	-0.561337
21	8	0	3.482034	0.946895	-0.217088
22	6	0	3.867168	-1.228579	-0.989874
23	6	0	4.557342	-0.011258	-0.302659
24	6	0	5.698403	0.602945	-1.087723
25	1	0	6.113755	1.452162	-0.530858
26	1	0	5.368630	0.969316	-2.065807
27	1	0	6.504539	-0.128387	-1.239678
28	6	0	5.007734	-0.301009	1.122323
29	1	0	5.280837	0.645692	1.604541
30	1	0	5.883536	-0.962466	1.143724
31	1	0	4.207599	-0.763245	1.715718
32	6	0	3.865327	-1.134996	-2.508832
33	1	0	4.867060	-1.299612	-2.926789
34	1	0	3.500855	-0.157834	-2.851358
35	1	0	3.194636	-1.904563	-2.910308
36	6	0	4.381507	-2.585309	-0.554877
37	1	0	5.450227	-2.689820	-0.788410
38	1	0	3.840805	-3.375240	-1.091192
39	1	0	4.240383	-2.749712	0.519180
40	6	0	-2.874949	2.813439	-0.549276
41	1	0	-3.716553	2.790605	0.157337
42	1	0	-3.277536	2.449041	-1.506705
43	6	0	-0.787196	4.049288	-0.750713
44	1	0	-0.216523	4.948458	-0.483889
45	1	0	-0.490333	3.752429	-1.769254
46	6	0	-2.300460	4.239310	-0.668786
47	6	0	-2.730625	-0.267122	-0.470873

48	6	0	-4.853850	-1.985897	-1.022917
49	6	0	-2.591765	-1.315713	-1.390680
50	6	0	-3.969997	-0.114316	0.163948
51	6	0	-5.035425	-0.966095	-0.103378
52	6	0	-3.645445	-2.175108	-1.674551
53	1	0	-1.641129	-1.457655	-1.903846
54	1	0	-4.092556	0.669913	0.909760
55	1	0	-5.995912	-0.856567	0.395183
56	1	0	-3.544905	-2.985618	-2.392896
57	6	0	0.780599	2.188772	0.052092
58	1	0	1.661353	2.824330	-0.071661
59	6	0	-0.278814	-0.044317	0.198917
60	1	0	-0.142593	-0.948867	-0.418523
61	1	0	-2.713680	4.792822	-1.520378
62	1	0	-2.543982	4.815276	0.236373
63	9	0	-5.872435	-2.814954	-1.286379

Zero-point correction= 0.533821
(Hartree/Particle)
Thermal correction to Energy= 0.564027
Thermal correction to Enthalpy= 0.564971
Thermal correction to Gibbs Free Energy= 0.474347
Sum of electronic and zero-point Energies= -1498.381787
Sum of electronic and thermal Energies= -1498.351581
Sum of electronic and thermal Enthalpies= -1498.350637
Sum of electronic and thermal Free Energies= -1498.441261

28cf



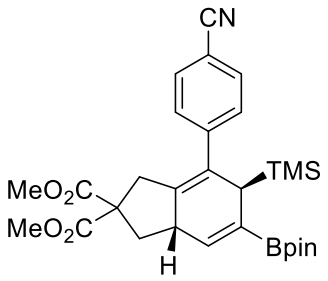
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542564	0.735552	-0.002086
2	6	0	-1.485529	-0.629179	-0.114160
3	6	0	0.757654	-1.723911	-0.049476
4	6	0	-0.607357	-1.718690	-0.705113
5	6	0	1.340761	-0.340414	-0.143374
6	6	0	-0.907369	0.543045	0.279843
7	1	0	0.640598	-1.996162	1.017405
8	1	0	-0.480802	-1.544019	-1.791693
9	1	0	-1.098340	-2.695741	-0.609096
10	14	0	-1.824794	1.850331	1.340924
11	6	0	-0.603065	2.920324	2.307939
12	1	0	-1.164638	3.401985	3.122154
13	1	0	-0.134482	3.714835	1.715079
14	1	0	0.195032	2.324720	2.772359
15	6	0	-2.792430	0.963643	2.692946
16	1	0	-3.543374	0.266946	2.310609
17	1	0	-3.308121	1.708124	3.316555
18	1	0	-2.103068	0.409457	3.344645
19	6	0	-2.924186	2.996541	0.329648
20	1	0	-3.525545	3.622965	1.003696

21	1	0	-3.607439	2.426764	-0.309767
22	1	0	-2.324073	3.668885	-0.298554
23	5	0	-3.010260	-0.938535	-0.169323
24	8	0	-4.026991	-0.015893	-0.142520
25	8	0	-3.469353	-2.212923	-0.399475
26	6	0	-5.275232	-0.743678	-0.165627
27	6	0	-4.851786	-2.103594	-0.799223
28	6	0	-4.866462	-2.086994	-2.321153
29	1	0	-4.356673	-2.985802	-2.688785
30	1	0	-4.338623	-1.210819	-2.719805
31	1	0	-5.890169	-2.087151	-2.716759
32	6	0	-5.609556	-3.311163	-0.288496
33	1	0	-5.240112	-4.215839	-0.787224
34	1	0	-6.682018	-3.217850	-0.508833
35	1	0	-5.484343	-3.446023	0.791126
36	6	0	-6.283145	0.051065	-0.969395
37	1	0	-7.225699	-0.505172	-1.067490
38	1	0	-5.910604	0.288303	-1.971496
39	1	0	-6.499492	0.996419	-0.455511
40	6	0	-5.754116	-0.879715	1.271853
41	1	0	-6.732181	-1.375511	1.321719
42	1	0	-5.855433	0.120182	1.712577
43	1	0	-5.044820	-1.453688	1.883250
44	6	0	2.793938	-0.412815	-0.534694
45	1	0	3.441846	0.225395	0.074711
46	1	0	2.922316	-0.094423	-1.582637
47	6	0	1.807762	-2.605963	-0.716329
48	1	0	1.796900	-3.653672	-0.394470
49	1	0	1.677462	-2.597307	-1.807167
50	6	0	3.153242	-1.909485	-0.408884
51	6	0	1.055304	2.104481	-0.230665
52	6	0	1.981868	4.707588	-0.690449
53	6	0	0.411779	2.940040	-1.152966
54	6	0	2.174152	2.596115	0.453420
55	6	0	2.639220	3.881466	0.230513
56	6	0	0.862531	4.230620	-1.383263
57	1	0	-0.455693	2.564329	-1.695708
58	1	0	2.653489	1.969226	1.204807
59	1	0	3.500644	4.262323	0.775228
60	1	0	0.359067	4.875075	-2.101012
61	6	0	2.452931	6.037590	-0.920729
62	7	0	2.837380	7.119970	-1.108202
63	6	0	4.216879	-2.338687	-1.423231
64	6	0	3.521058	-2.254788	1.023214
65	8	0	3.937242	-2.952209	-2.422434
66	8	0	3.383993	-1.528211	1.979600
67	8	0	5.494473	-1.956291	-1.254313
68	8	0	3.980476	-3.510731	1.098987
69	6	0	5.998047	-1.311054	-0.094512
70	1	0	5.352111	-0.499378	0.254914
71	1	0	6.962505	-0.888638	-0.386080
72	1	0	6.160716	-2.034936	0.713497
73	6	0	4.324231	-3.961452	2.410358
74	1	0	4.716373	-4.971750	2.286658
75	1	0	3.439894	-3.966885	3.055439
76	1	0	5.082688	-3.305789	2.852546

Zero-point correction= 0.627095
(Hartree/Particle)
Thermal correction to Energy= 0.667019
Thermal correction to Enthalpy= 0.667964

Thermal correction to Gibbs Free Energy= 0.554961
Sum of electronic and zero-point Energies= -1946.761533
Sum of electronic and thermal Energies= -1946.721608
Sum of electronic and thermal Enthalpies= -1946.720664
Sum of electronic and thermal Free Energies= -1946.833667

26cf

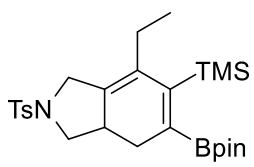


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440102	0.857318	0.037731
2	6	0	-1.567941	-0.663683	0.071370
3	6	0	0.715969	-1.607043	0.385733
4	6	0	1.239516	-0.219607	0.120013
5	1	0	0.950386	-1.888523	1.432527
6	14	0	-1.435863	1.310768	2.085123
7	6	0	-0.245229	0.480805	3.283089
8	1	0	-0.469805	0.787916	4.313572
9	1	0	0.803967	0.731658	3.078413
10	1	0	-0.346796	-0.612245	3.236243
11	6	0	-3.189253	0.808618	2.551434
12	1	0	-3.921624	1.155961	1.811730
13	1	0	-3.455490	1.228405	3.530971
14	1	0	-3.270684	-0.285458	2.624279
15	6	0	-1.282668	3.186038	2.175092
16	1	0	-1.568656	3.544460	3.173527
17	1	0	-1.950092	3.665953	1.445952
18	1	0	-0.261556	3.535804	1.972112
19	5	0	-3.061429	-0.871474	-0.288207
20	8	0	-3.923275	0.164641	-0.548309
21	8	0	-3.653126	-2.102867	-0.406355
22	6	0	-5.134005	-0.418798	-1.079511
23	6	0	-5.073918	-1.874276	-0.523624
24	6	0	-5.668059	-2.930072	-1.432637
25	1	0	-5.576516	-3.916175	-0.960259
26	1	0	-5.156701	-2.971782	-2.400213
27	1	0	-6.735651	-2.737104	-1.607212
28	6	0	-5.655558	-2.009007	0.876603
29	1	0	-5.383662	-2.993577	1.276378
30	1	0	-6.750327	-1.930921	0.872252
31	1	0	-5.254786	-1.245470	1.556723
32	6	0	-5.023686	-0.352329	-2.595814
33	1	0	-5.941836	-0.703542	-3.083907
34	1	0	-4.181060	-0.951002	-2.965470
35	1	0	-4.854832	0.690047	-2.892769
36	6	0	-6.320124	0.397466	-0.610257
37	1	0	-7.262718	-0.068651	-0.929329
38	1	0	-6.274348	1.401033	-1.051428
39	1	0	-6.336806	0.508379	0.479573
40	6	0	2.714742	-0.318228	-0.180114
41	1	0	3.319876	0.013110	0.674947

42	1	0	3.003177	0.298708	-1.044159
43	6	0	1.581042	-2.457842	-0.545614
44	1	0	1.581340	-3.530051	-0.313700
45	1	0	1.238147	-2.343238	-1.581928
46	6	0	2.987966	-1.827903	-0.435476
47	6	0	0.960162	2.210678	-0.251521
48	6	0	1.897653	4.812782	-0.733237
49	6	0	0.327439	3.041624	-1.187909
50	6	0	2.071708	2.715815	0.438052
51	6	0	2.540325	3.999439	0.206788
52	6	0	0.787717	4.324339	-1.433744
53	1	0	-0.533352	2.670486	-1.741768
54	1	0	2.551575	2.100150	1.197216
55	1	0	3.395742	4.384618	0.757861
56	1	0	0.294494	4.958029	-2.167807
57	6	0	2.370948	6.139904	-0.974466
58	7	0	2.757259	7.220104	-1.170442
59	6	0	3.779305	-2.065171	-1.724169
60	6	0	3.651077	-2.475021	0.769716
61	8	0	3.284827	-2.544025	-2.713044
62	8	0	3.706127	-2.003108	1.881223
63	8	0	5.061991	-1.663083	-1.787642
64	8	0	4.121427	-3.687771	0.451243
65	6	0	5.797808	-1.181017	-0.673874
66	1	0	5.271361	-0.389785	-0.129095
67	1	0	6.720188	-0.765535	-1.086410
68	1	0	6.057672	-1.998963	0.009554
69	6	0	4.718363	-4.417423	1.524588
70	1	0	5.061541	-5.358386	1.092528
71	1	0	3.984195	-4.600947	2.315459
72	1	0	5.561577	-3.857634	1.944603
73	6	0	-0.752356	-1.728185	0.142377
74	1	0	-1.153974	-2.731894	-0.016130
75	6	0	-1.040668	0.725904	0.290648
76	1	0	-1.599594	1.431012	-0.346962

Zero-point correction= 0.626897
(Hartree/Particle)
Thermal correction to Energy= 0.666820
Thermal correction to Enthalpy= 0.667764
Thermal correction to Gibbs Free Energy= 0.554550
Sum of electronic and zero-point Energies= -1946.769881
Sum of electronic and thermal Energies= -1946.729958
Sum of electronic and thermal Enthalpies= -1946.729014
Sum of electronic and thermal Free Energies= -1946.842228

28bo



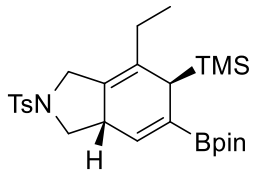
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.121047	1.722351	0.331408
2	6	0	1.700994	-0.025576	-0.336652
3	6	0	-0.529897	0.104939	-1.439252
4	6	0	-0.832962	1.216638	-0.470097
5	1	0	-0.140128	0.516731	-2.388166

6	14	0	2.990292	2.405755	0.523932
7	6	0	2.458735	4.219079	0.425853
8	1	0	3.376684	4.824942	0.434554
9	1	0	1.830251	4.569531	1.252394
10	1	0	1.939741	4.439622	-0.517458
11	6	0	4.317279	2.263834	-0.819084
12	1	0	5.251746	1.870583	-0.401963
13	1	0	4.519905	3.256865	-1.242634
14	1	0	4.017255	1.606869	-1.644159
15	6	0	3.717515	2.111750	2.237059
16	1	0	4.546368	2.810843	2.417286
17	1	0	4.105777	1.089616	2.319471
18	1	0	2.972811	2.268080	3.028995
19	5	0	3.023787	-0.834923	-0.286315
20	8	0	4.183828	-0.447568	0.336280
21	8	0	3.098199	-2.117209	-0.777624
22	6	0	5.177678	-1.457762	0.059239
23	6	0	4.296763	-2.708773	-0.233073
24	6	0	3.882437	-3.459253	1.025001
25	1	0	3.102676	-4.184274	0.761568
26	1	0	3.470575	-2.779604	1.782266
27	1	0	4.724662	-4.006702	1.467643
28	6	0	4.871719	-3.677944	-1.244611
29	1	0	4.181021	-4.519474	-1.380414
30	1	0	5.831419	-4.081970	-0.893255
31	1	0	5.025076	-3.207638	-2.221617
32	6	0	6.089503	-1.572553	1.262803
33	1	0	6.824972	-2.377049	1.123341
34	1	0	5.528526	-1.764730	2.183981
35	1	0	6.638247	-0.630506	1.393583
36	6	0	5.974519	-1.000539	-1.154224
37	1	0	6.778979	-1.707980	-1.392364
38	1	0	6.431530	-0.026081	-0.943455
39	1	0	5.333939	-0.888323	-2.038978
40	6	0	-2.304582	1.512940	-0.486339
41	1	0	-2.555681	2.549784	-0.739892
42	1	0	-2.768572	1.287945	0.496753
43	6	0	-1.897336	-0.526066	-1.679627
44	1	0	-2.016890	-0.988012	-2.664248
45	1	0	-2.101961	-1.286762	-0.899741
46	7	0	-2.800216	0.623752	-1.549378
47	6	0	1.516594	1.233639	0.160321
48	6	0	-0.214558	2.662175	1.469010
49	1	0	0.693861	2.870003	2.050455
50	1	0	-0.878128	2.122720	2.166004
51	6	0	-0.881741	3.981183	1.086115
52	1	0	-0.353777	4.478044	0.263332
53	1	0	-0.896684	4.668769	1.941414
54	1	0	-1.922468	3.840746	0.771391
55	16	0	-4.439679	0.374083	-1.651593
56	8	0	-5.058507	1.687726	-1.536680
57	8	0	-4.654046	-0.473456	-2.816050
58	6	0	-4.880791	-0.560687	-0.207817
59	6	0	-5.449950	-2.024464	2.097327
60	6	0	-5.270039	0.107017	0.952041
61	6	0	-4.772995	-1.950129	-0.231471
62	6	0	-5.057621	-2.670462	0.921059
63	6	0	-5.551809	-0.630537	2.094610
64	1	0	-5.372562	1.190407	0.943693
65	1	0	-4.492322	-2.456877	-1.153116
66	1	0	-4.980670	-3.757600	0.909487

67	1	0	-5.862536	-0.116381	3.004158
68	6	0	-5.786041	-2.812954	3.326310
69	1	0	-5.230160	-3.757423	3.363494
70	1	0	-6.855520	-3.064748	3.350730
71	1	0	-5.565398	-2.248492	4.240287
72	6	0	0.494277	-0.813470	-0.809192
73	1	0	0.027154	-1.323792	0.055958
74	1	0	0.805427	-1.607417	-1.500842

Zero-point correction= 0.626836
(Hartree/Particle)
Thermal correction to Energy= 0.663328
Thermal correction to Enthalpy= 0.664272
Thermal correction to Gibbs Free Energy= 0.559864
Sum of electronic and zero-point Energies= -2081.431853
Sum of electronic and thermal Energies= -2081.395361
Sum of electronic and thermal Enthalpies= -2081.394417
Sum of electronic and thermal Free Energies= -2081.498825

26bo



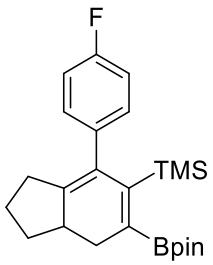
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.096910	-1.677364	0.893855
2	6	0	-1.704192	-0.215934	-0.377867
3	6	0	0.420936	-0.940924	-1.447862
4	6	0	0.780950	-1.535058	-0.107786
5	1	0	0.283730	-1.747029	-2.195391
6	14	0	-2.624425	-2.785956	0.239702
7	6	0	-1.829045	-3.735957	-1.175927
8	1	0	-2.436716	-4.611827	-1.440144
9	1	0	-0.819260	-4.086003	-0.925043
10	1	0	-1.755710	-3.101856	-2.070596
11	6	0	-4.322381	-2.187099	-0.306479
12	1	0	-4.767491	-1.518095	0.441232
13	1	0	-5.001143	-3.038553	-0.451305
14	1	0	-4.264117	-1.641181	-1.258742
15	6	0	-2.849979	-3.885968	1.753873
16	1	0	-3.521611	-4.722180	1.515527
17	1	0	-3.305606	-3.320365	2.578615
18	1	0	-1.907748	-4.312746	2.120864
19	5	0	-2.872403	0.800877	-0.296642
20	8	0	-3.654241	0.971316	0.818199
21	8	0	-3.184079	1.676896	-1.306489
22	6	0	-4.678948	1.933034	0.477283
23	6	0	-4.039951	2.685505	-0.730655
24	6	0	-3.138835	3.837586	-0.308935
25	1	0	-2.565209	4.174418	-1.181115
26	1	0	-2.424850	3.527209	0.465157
27	1	0	-3.717770	4.688785	0.071740
28	6	0	-5.022636	3.155744	-1.783201
29	1	0	-4.481183	3.661861	-2.592179
30	1	0	-5.738418	3.871875	-1.356137
31	1	0	-5.581555	2.321440	-2.220796

32	6	0	-4.960218	2.795322	1.690464
33	1	0	-5.672237	3.594800	1.442798
34	1	0	-4.046640	3.250584	2.087536
35	1	0	-5.404927	2.181651	2.483900
36	6	0	-5.925501	1.148902	0.098289
37	1	0	-6.777703	1.814725	-0.089482
38	1	0	-6.192483	0.480880	0.927047
39	1	0	-5.760013	0.534083	-0.795593
40	6	0	2.269594	-1.743719	-0.065179
41	1	0	2.586014	-2.795089	-0.095805
42	1	0	2.712825	-1.290948	0.842537
43	6	0	1.695628	-0.182910	-1.818187
44	1	0	1.834943	-0.028330	-2.892978
45	1	0	1.707496	0.798712	-1.305940
46	7	0	2.735082	-1.077976	-1.298497
47	6	0	-0.802771	-0.087683	-1.366374
48	1	0	-0.934504	0.685196	-2.127332
49	6	0	-1.530051	-1.268706	0.683552
50	1	0	-1.947737	-0.898134	1.636330
51	6	0	0.290911	-2.207934	2.253529
52	1	0	-0.594551	-2.199865	2.906959
53	1	0	1.008133	-1.512127	2.721649
54	6	0	0.891906	-3.610834	2.250495
55	1	0	0.232549	-4.327406	1.741210
56	1	0	1.051126	-3.970701	3.274756
57	1	0	1.861286	-3.645373	1.738338
58	16	0	4.318823	-0.589351	-1.371683
59	8	0	5.113306	-1.701638	-0.867952
60	8	0	4.520165	-0.049301	-2.709417
61	6	0	4.473897	0.751416	-0.217455
62	6	0	4.605656	2.843344	1.623269
63	6	0	4.840700	0.486224	1.100168
64	6	0	4.174473	2.049548	-0.628939
65	6	0	4.242455	3.083878	0.294100
66	6	0	4.902939	1.534264	2.009958
67	1	0	5.099496	-0.529269	1.394024
68	1	0	3.918594	2.243142	-1.669094
69	1	0	4.016059	4.102788	-0.020491
70	1	0	5.194893	1.335532	3.041125
71	6	0	4.707957	3.973950	2.601178
72	1	0	3.928332	4.726741	2.431295
73	1	0	5.675836	4.486118	2.507798
74	1	0	4.624383	3.621041	3.635781

Zero-point correction= 0.625347
(Hartree/Particle)
Thermal correction to Energy= 0.662272
Thermal correction to Enthalpy= 0.663216
Thermal correction to Gibbs Free Energy= 0.557489
Sum of electronic and zero-point Energies= -2081.443585
Sum of electronic and thermal Energies= -2081.406660
Sum of electronic and thermal Enthalpies= -2081.405716
Sum of electronic and thermal Free Energies= -2081.511443

CARTESIAN COORDINATES – B3LYP

28ec

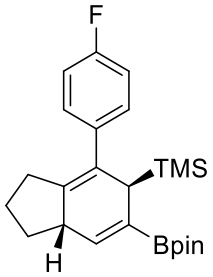


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.651949	0.768721	-0.159398
2	6	0	-0.805953	0.808817	0.018606
3	6	0	0.465590	2.947407	-0.355642
4	6	0	-0.649940	2.275329	0.435123
5	6	0	1.730438	2.117938	-0.219103
6	6	0	0.315999	0.100375	-0.322387
7	1	0	0.169578	2.993341	-1.418952
8	1	0	-0.407698	2.328161	1.511379
9	1	0	-1.598729	2.804952	0.304870
10	14	0	0.232222	-1.615843	-1.196916
11	6	0	1.798915	-1.938207	-2.223975
12	1	0	1.587462	-2.760613	-2.920281
13	1	0	2.665543	-2.224125	-1.622512
14	1	0	2.081369	-1.066021	-2.825691
15	6	0	-1.164752	-1.599827	-2.485012
16	1	0	-2.155417	-1.521780	-2.032467
17	1	0	-1.133368	-2.530532	-3.066466
18	1	0	-1.037603	-0.768238	-3.188933
19	6	0	-0.002732	-3.057482	0.010607
20	1	0	-0.115070	-3.999229	-0.542263
21	1	0	-0.899129	-2.909938	0.619682
22	1	0	0.860355	-3.164522	0.677185
23	5	0	-2.266675	0.275094	0.134501
24	8	0	-2.649161	-1.032251	0.348417
25	8	0	-3.342100	1.138190	0.149138
26	6	0	-4.053591	-1.033701	0.741569
27	6	0	-4.562162	0.346305	0.171257
28	6	0	-5.591388	1.069096	1.039383
29	1	0	-5.847702	2.029415	0.580294
30	1	0	-5.208305	1.266416	2.043156
31	1	0	-6.511341	0.479840	1.125568
32	6	0	-5.064087	0.265748	-1.277359
33	1	0	-5.214504	1.281197	-1.657028
34	1	0	-6.016151	-0.270936	-1.344257
35	1	0	-4.338200	-0.232290	-1.927757
36	6	0	-4.076069	-1.105684	2.274648
37	1	0	-5.099217	-1.168915	2.659600
38	1	0	-3.589582	-0.232987	2.721805
39	1	0	-3.531753	-1.998835	2.596974
40	6	0	-4.726245	-2.270849	0.149646
41	1	0	-5.796892	-2.278275	0.383460
42	1	0	-4.280581	-3.173661	0.579767
43	1	0	-4.607394	-2.318997	-0.935144
44	6	0	2.926941	3.037498	-0.028269
45	1	0	3.777615	2.796211	-0.671878
46	1	0	3.294196	2.960220	1.005992

47	6	0	0.888033	4.355734	0.111427
48	1	0	0.265970	5.150799	-0.313192
49	1	0	0.803655	4.419493	1.205385
50	6	0	2.367276	4.451668	-0.303696
51	1	0	2.915886	5.236302	0.227611
52	1	0	2.436598	4.673972	-1.376609
53	6	0	2.844272	-0.062168	0.184678
54	6	0	5.059913	-1.595670	0.934900
55	6	0	2.782583	-0.940332	1.281519
56	6	0	4.055066	0.018362	-0.523587
57	6	0	5.165883	-0.741197	-0.156626
58	6	0	3.882092	-1.710223	1.663435
59	1	0	1.861009	-1.012608	1.851938
60	1	0	4.123089	0.664697	-1.392855
61	1	0	6.099065	-0.685582	-0.707982
62	1	0	3.837423	-2.383384	2.513579
63	9	0	6.132664	-2.336741	1.296604

Zero-point correction= 0.535104
(Hartree/Particle)
Thermal correction to Energy= 0.565977
Thermal correction to Enthalpy= 0.566921
Thermal correction to Gibbs Free Energy= 0.474200
Sum of electronic and zero-point Energies= -1499.245087
Sum of electronic and thermal Energies= -1499.214214
Sum of electronic and thermal Enthalpies= -1499.213270
Sum of electronic and thermal Free Energies= -1499.305991

26ec

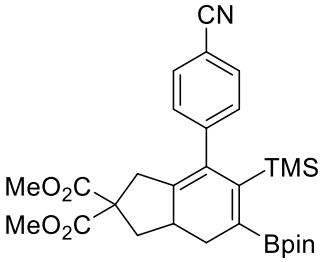


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.605944	0.563285	-0.096281
2	6	0	0.907751	0.843983	0.021385
3	6	0	-0.577529	2.856465	-0.056782
4	6	0	-1.734657	1.890955	-0.284395
5	1	0	-0.668329	3.307506	0.948723
6	14	0	-0.329184	-0.321231	2.323677
7	6	0	-0.852290	1.253309	3.240452
8	1	0	-0.902897	1.067015	4.320612
9	1	0	-1.838171	1.602727	2.914078
10	1	0	-0.135221	2.066310	3.078293
11	6	0	1.387729	-0.840052	2.940755
12	1	0	1.781780	-1.687886	2.370430
13	1	0	1.336175	-1.134009	3.996848
14	1	0	2.110359	-0.019218	2.861413
15	6	0	-1.550655	-1.718628	2.712683
16	1	0	-1.560817	-1.927350	3.790166
17	1	0	-1.270309	-2.646233	2.198738
18	1	0	-2.573058	-1.470017	2.408855
19	5	0	2.289176	0.188080	-0.252419

20	8	0	2.486773	-1.174987	-0.295805
21	8	0	3.437299	0.899484	-0.521123
22	6	0	3.817647	-1.411784	-0.840830
23	6	0	4.546906	-0.042767	-0.549543
24	6	0	5.536416	0.408647	-1.622635
25	1	0	5.958258	1.380498	-1.346261
26	1	0	5.055660	0.514735	-2.597837
27	1	0	6.363530	-0.304434	-1.715633
28	6	0	5.209625	0.014000	0.833842
29	1	0	5.513089	1.045395	1.039399
30	1	0	6.099783	-0.621985	0.882243
31	1	0	4.516642	-0.298022	1.621655
32	6	0	3.634474	-1.698938	-2.337644
33	1	0	4.586027	-1.946239	-2.819747
34	1	0	3.194103	-0.842249	-2.857650
35	1	0	2.957779	-2.551127	-2.456185
36	6	0	4.418647	-2.631260	-0.144252
37	1	0	5.443398	-2.810101	-0.489243
38	1	0	3.823464	-3.519491	-0.380290
39	1	0	4.432396	-2.512501	0.941539
40	6	0	-2.892867	2.651983	-0.922575
41	1	0	-3.812006	2.620941	-0.327722
42	1	0	-3.145323	2.210049	-1.895990
43	6	0	-0.844284	3.978801	-1.086912
44	1	0	-0.332312	4.915579	-0.840679
45	1	0	-0.492185	3.655292	-2.075669
46	6	0	-2.377465	4.104749	-1.081317
47	6	0	-2.704535	-0.393884	-0.416636
48	6	0	-4.760595	-2.187162	-1.043630
49	6	0	-2.477405	-1.494508	-1.263710
50	6	0	-3.998134	-0.232017	0.110367
51	6	0	-5.029988	-1.120074	-0.195706
52	6	0	-3.496907	-2.389799	-1.585943
53	1	0	-1.491631	-1.646495	-1.693936
54	1	0	-4.196742	0.594593	0.785460
55	1	0	-6.025988	-0.997905	0.217730
56	1	0	-3.324192	-3.232779	-2.247345
57	6	0	0.755478	2.169096	-0.169519
58	1	0	1.612871	2.779054	-0.451604
59	6	0	-0.286706	-0.011181	0.407505
60	1	0	-0.149809	-1.017657	-0.010166
61	1	0	-2.770803	4.595830	-1.977366
62	1	0	-2.690821	4.706667	-0.218528
63	9	0	-5.753649	-3.054995	-1.346705

Zero-point correction= 0.534729
(Hartree/Particle)
Thermal correction to Energy= 0.565752
Thermal correction to Enthalpy= 0.566696
Thermal correction to Gibbs Free Energy= 0.472867
Sum of electronic and zero-point Energies= -1499.251317
Sum of electronic and thermal Energies= -1499.220294
Sum of electronic and thermal Enthalpies= -1499.219350
Sum of electronic and thermal Free Energies= -1499.313179

28cf

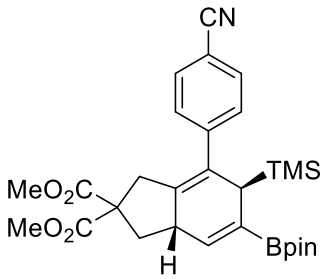


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534283	0.779306	0.092753
2	6	0	-1.520291	-0.564299	-0.097427
3	6	0	0.730560	-1.694313	-0.015187
4	6	0	-0.627652	-1.648351	-0.707920
5	6	0	1.332017	-0.306451	-0.024795
6	6	0	-0.936153	0.594600	0.341847
7	1	0	0.593155	-2.028807	1.026590
8	1	0	-0.476404	-1.439311	-1.781321
9	1	0	-1.128158	-2.619173	-0.653003
10	14	0	-1.859538	1.882344	1.445312
11	6	0	-0.640125	2.951511	2.435725
12	1	0	-1.204755	3.434742	3.244290
13	1	0	-0.164473	3.741158	1.848392
14	1	0	0.150944	2.354597	2.904624
15	6	0	-2.834342	0.952582	2.780438
16	1	0	-3.581891	0.272136	2.370905
17	1	0	-3.352704	1.674554	3.425063
18	1	0	-2.153068	0.374670	3.417078
19	6	0	-2.977716	3.038199	0.443840
20	1	0	-3.540952	3.696004	1.118553
21	1	0	-3.692948	2.467825	-0.154510
22	1	0	-2.389358	3.677209	-0.224888
23	5	0	-3.045976	-0.894643	-0.184983
24	8	0	-4.093863	-0.003672	-0.123741
25	8	0	-3.468276	-2.172440	-0.483100
26	6	0	-5.342214	-0.755095	-0.221547
27	6	0	-4.866687	-2.108632	-0.880346
28	6	0	-4.884216	-2.082027	-2.415232
29	1	0	-4.362696	-2.967559	-2.791570
30	1	0	-4.372049	-1.196747	-2.805472
31	1	0	-5.906530	-2.092719	-2.806839
32	6	0	-5.572281	-3.364761	-0.371554
33	1	0	-5.149864	-4.246612	-0.863975
34	1	0	-6.643236	-3.330518	-0.601020
35	1	0	-5.450526	-3.489899	0.706778
36	6	0	-6.327578	0.061735	-1.056101
37	1	0	-7.258749	-0.494909	-1.210835
38	1	0	-5.912623	0.324445	-2.031767
39	1	0	-6.573056	0.990314	-0.530632
40	6	0	-5.883731	-0.927774	1.203156
41	1	0	-6.852798	-1.437465	1.201515
42	1	0	-6.018019	0.058449	1.657874
43	1	0	-5.193596	-1.500798	1.830218
44	6	0	2.820761	-0.377414	-0.314707
45	1	0	3.415151	0.131417	0.445610
46	1	0	3.054136	0.093844	-1.278473
47	6	0	1.789115	-2.561059	-0.715667

48	1	0	1.755811	-3.616899	-0.434615
49	1	0	1.672254	-2.508617	-1.801861
50	6	0	3.157555	-1.900610	-0.362175
51	6	0	1.065047	2.150907	-0.149798
52	6	0	2.061317	4.726212	-0.729603
53	6	0	0.445901	2.967003	-1.115279
54	6	0	2.191957	2.657893	0.521343
55	6	0	2.689015	3.925703	0.240774
56	6	0	0.931186	4.236962	-1.407495
57	1	0	-0.420413	2.590790	-1.650982
58	1	0	2.664115	2.064368	1.297305
59	1	0	3.553657	4.306538	0.774897
60	1	0	0.447167	4.850607	-2.160493
61	6	0	2.569452	6.032963	-1.023952
62	7	0	2.983358	7.094252	-1.263232
63	6	0	4.206146	-2.237571	-1.445268
64	6	0	3.554278	-2.409901	1.025922
65	8	0	3.905473	-2.785743	-2.481557
66	8	0	3.384087	-1.810867	2.067365
67	8	0	5.493500	-1.847557	-1.296904
68	8	0	4.063626	-3.654416	0.952462
69	6	0	6.051241	-1.295603	-0.097490
70	1	0	5.411849	-0.534387	0.352700
71	1	0	6.991121	-0.833606	-0.403350
72	1	0	6.259931	-2.088955	0.625751
73	6	0	4.377137	-4.286273	2.210401
74	1	0	4.793318	-5.258720	1.949864
75	1	0	3.471112	-4.401910	2.809988
76	1	0	5.104800	-3.690531	2.766617

Zero-point correction= 0.627588
(Hartree/Particle)
Thermal correction to Energy= 0.668578
Thermal correction to Enthalpy= 0.669522
Thermal correction to Gibbs Free Energy= 0.552844
Sum of electronic and zero-point Energies= -1947.886036
Sum of electronic and thermal Energies= -1947.845046
Sum of electronic and thermal Enthalpies= -1947.844102
Sum of electronic and thermal Free Energies= -1947.960780

26cf



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.405604	0.868409	0.215696
2	6	0	-1.592525	-0.682691	0.170931
3	6	0	0.716958	-1.617205	0.416913
4	6	0	1.223285	-0.202787	0.201111
5	1	0	0.929518	-1.930272	1.453902
6	14	0	-1.426884	1.079745	2.416434
7	6	0	-0.326598	0.014092	3.529931

8	1	0	-0.517451	0.248052	4.584812
9	1	0	0.738738	0.183217	3.338326
10	1	0	-0.529540	-1.053559	3.387255
11	6	0	-3.243071	0.708379	2.810317
12	1	0	-3.919806	1.214717	2.114045
13	1	0	-3.483853	1.045299	3.826480
14	1	0	-3.453653	-0.366313	2.760150
15	6	0	-1.101737	2.916195	2.758124
16	1	0	-1.374781	3.159444	3.792868
17	1	0	-1.699877	3.557732	2.099618
18	1	0	-0.049998	3.188011	2.618795
19	5	0	-3.071342	-0.864331	-0.275842
20	8	0	-3.925059	0.191810	-0.498662
21	8	0	-3.650199	-2.084506	-0.535139
22	6	0	-5.114776	-0.333048	-1.159624
23	6	0	-5.071943	-1.861980	-0.765523
24	6	0	-5.541016	-2.826597	-1.853642
25	1	0	-5.440564	-3.857107	-1.497774
26	1	0	-4.950166	-2.726067	-2.766883
27	1	0	-6.595328	-2.654999	-2.098508
28	6	0	-5.785717	-2.173989	0.556794
29	1	0	-5.544671	-3.198820	0.856299
30	1	0	-6.873141	-2.092050	0.457799
31	1	0	-5.458285	-1.502347	1.356675
32	6	0	-4.925072	-0.084096	-2.662189
33	1	0	-5.803703	-0.395857	-3.236260
34	1	0	-4.050910	-0.618242	-3.047775
35	1	0	-4.768672	0.986400	-2.828407
36	6	0	-6.331761	0.436430	-0.649602
37	1	0	-7.254935	0.034933	-1.082400
38	1	0	-6.251117	1.488146	-0.943383
39	1	0	-6.410897	0.394366	0.439086
40	6	0	2.692402	-0.257265	-0.183214
41	1	0	3.328847	0.092818	0.634662
42	1	0	2.906540	0.368845	-1.056654
43	6	0	1.604347	-2.445717	-0.533976
44	1	0	1.646652	-3.509918	-0.285316
45	1	0	1.241884	-2.361052	-1.561591
46	6	0	3.006716	-1.765865	-0.467003
47	6	0	0.888931	2.234732	-0.124998
48	6	0	1.808057	4.816339	-0.810288
49	6	0	0.216676	3.013541	-1.087072
50	6	0	2.027327	2.787985	0.490519
51	6	0	2.485932	4.058760	0.159347
52	6	0	0.666988	4.281580	-1.434085
53	1	0	-0.658789	2.611462	-1.587408
54	1	0	2.546419	2.221342	1.256748
55	1	0	3.360612	4.471771	0.651578
56	1	0	0.144282	4.861724	-2.187730
57	6	0	2.274403	6.125311	-1.158618
58	7	0	2.654237	7.188537	-1.441843
59	6	0	3.757383	-1.965333	-1.802019
60	6	0	3.748103	-2.399892	0.714691
61	8	0	3.235103	-2.467397	-2.771110
62	8	0	3.813563	-1.934807	1.833773
63	8	0	5.021459	-1.500498	-1.943252
64	8	0	4.268907	-3.592723	0.370411
65	6	0	5.827048	-0.998237	-0.869152
66	1	0	5.293614	-0.278623	-0.245116
67	1	0	6.666852	-0.495800	-1.351412
68	1	0	6.205972	-1.821786	-0.257332

69	6	0	4.902707	-4.337609	1.430394
70	1	0	5.272590	-5.248958	0.962050
71	1	0	4.176992	-4.572278	2.212696
72	1	0	5.725686	-3.762437	1.861375
73	6	0	-0.758089	-1.738962	0.143184
74	1	0	-1.136254	-2.723713	-0.126867
75	6	0	-1.070412	0.693019	0.543248
76	1	0	-1.656488	1.451341	0.008292

Zero-point correction= 0.627262
(Hartree/Particle)
Thermal correction to Energy= 0.668339
Thermal correction to Enthalpy= 0.669283
Thermal correction to Gibbs Free Energy= 0.551648
Sum of electronic and zero-point Energies= -1947.894119
Sum of electronic and thermal Energies= -1947.853043
Sum of electronic and thermal Enthalpies= -1947.852098
Sum of electronic and thermal Free Energies= -1947.969733