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SUPPORTING INFORMATION

On the mechanism of the formation of alkyl-Ni(I) catalysts

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I. Computational results

I.1. 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, F 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 THF or diisopropylether using the polarized continuum model (PCM). Gibbs free energies were also calculated by single points calculations using the M06 functional to assess the reliability of the results.

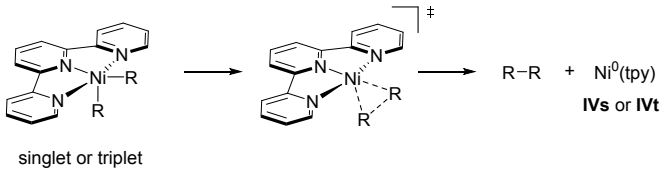
This ESI includes computational results in gas phase (which are not included in the main manuscript), along with the results in THF and diisopropylether for the different processes studied.

[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.

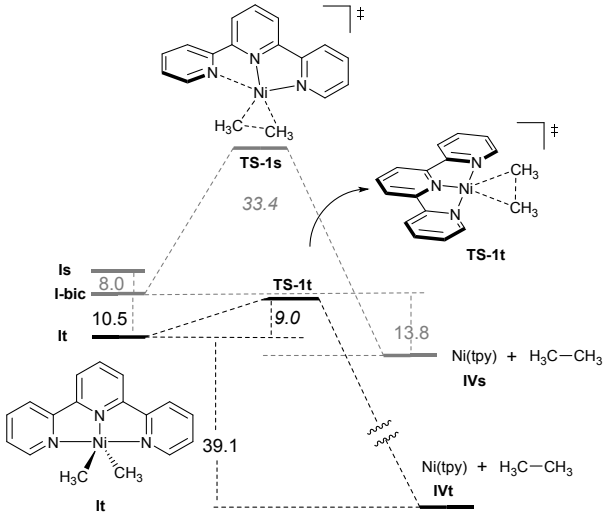
[2] Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, *120*: 215–241.

[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.

I.2. Atomic coordinates and energies for the stationary points in gas phase



	I-bic R = CH_3 singlet	**It** R = CH_3 triplet	**IIs** singlet	**IIt** triplet	**IIIs** R = CF_3 singlet	**IIIt** R = CF_3 triplet
ΔG_a	33.4	9.0	44.3	17.0	-	46.7
ΔG	-13.8	-39.1	19.0	-6.3	15.9	-11.4



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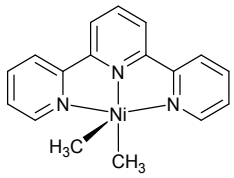
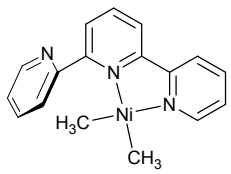


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.479452	-0.569301	5.669101
2	6	0	0.188427	-0.208002	4.687948
3	7	0	-0.562534	0.696119	2.164066
4	6	0	1.070158	-0.298314	3.616859
5	6	0	-1.074383	0.334310	4.475740
6	6	0	-1.404243	0.766546	3.193340
7	6	0	0.654096	0.167428	2.370011
8	1	0	2.049190	-0.749403	3.739110
9	1	0	-1.796012	0.416773	5.280801
10	1	0	-2.384661	1.179934	2.971637
11	6	0	1.512671	0.090912	1.160598
12	6	0	2.907183	0.087225	-1.201109
13	6	0	2.907183	0.087225	1.201109
14	7	0	0.848242	0.060984	-0.000000

15	6	0	1.512671	0.090912	-1.160598
16	6	0	3.607085	0.072172	-0.000000
17	1	0	3.430198	0.130516	2.149938
18	1	0	4.692247	0.083529	-0.000000
19	1	0	3.430198	0.130516	-2.149938
20	6	0	0.654096	0.167428	-2.370011
21	6	0	-1.074383	0.334310	-4.475740
22	6	0	1.070158	-0.298314	-3.616859
23	7	0	-0.562534	0.696119	-2.164066
24	6	0	-1.404243	0.766546	-3.193340
25	6	0	0.188427	-0.208002	-4.687948
26	1	0	2.049190	-0.749403	-3.739110
27	1	0	-2.384661	1.179934	-2.971637
28	1	0	0.479452	-0.569301	-5.669101
29	1	0	-1.796012	0.416773	-5.280801
30	28	0	-1.207062	-0.101563	0.000000
31	6	0	-3.126436	-0.039233	0.000000
32	1	0	-3.577026	-0.503640	-0.886436
33	1	0	-3.401027	1.033398	0.000000
34	1	0	-3.577026	-0.503640	0.886436
35	6	0	-1.228298	-2.064436	0.000000
36	1	0	-0.208956	-2.479363	0.000000
37	1	0	-1.755021	-2.434189	-0.887223
38	1	0	-1.755021	-2.434189	0.887223

Zero-point correction= 0.302388
(Hartree/Particle)
Thermal correction to Energy= 0.320815
Thermal correction to Enthalpy= 0.321759
Thermal correction to Gibbs Free Energy= 0.255436
Sum of electronic and zero-point Energies= -990.901367
Sum of electronic and thermal Energies= -990.882941
Sum of electronic and thermal Enthalpies= -990.881996
Sum of electronic and thermal Free Energies= -990.948320

I-bic



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.625156	0.146898	0.718336
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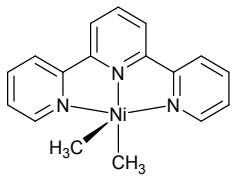
3	7	0	-2.284454	-0.312347	-1.198467
4	6	0	-3.595617	0.824203	0.466723
5	6	0	-4.567380	-0.947889	-0.810327
6	6	0	-3.344589	-1.069389	-1.468859
7	6	0	-2.411728	0.606967	-0.238294
8	1	0	-3.638677	1.573296	1.251200
9	1	0	-5.394235	-1.600734	-1.067274
10	1	0	-3.209451	-1.813406	-2.249581
11	6	0	-1.197186	1.426590	0.023547
12	6	0	1.108229	2.897387	0.208654
13	6	0	-1.284698	2.812468	0.168724
14	7	0	-0.018521	0.794039	0.032279
15	6	0	1.115749	1.509506	0.066328

16	6	0	-0.114948	3.550479	0.286812
17	1	0	-2.255641	3.295383	0.151314
18	1	0	-0.152903	4.629043	0.401006
19	1	0	2.031887	3.461293	0.250790
20	6	0	2.361893	0.714675	-0.112647
21	6	0	4.532342	-0.897429	-0.551860
22	6	0	3.633063	1.285765	-0.150562
23	7	0	2.176042	-0.607374	-0.274904
24	6	0	3.233299	-1.391479	-0.482901
25	6	0	4.732365	0.465952	-0.376046
26	1	0	3.770194	2.351102	-0.009742
27	1	0	3.017542	-2.450242	-0.582204
28	1	0	5.730651	0.890064	-0.413837
29	1	0	5.360087	-1.573647	-0.732027
30	28	0	0.305899	-1.252528	0.365763
31	6	0	0.796872	-3.124306	0.486896
32	1	0	1.603567	-3.268706	1.222223
33	1	0	1.169630	-3.455015	-0.498462
34	1	0	-0.029780	-3.784085	0.764653
35	6	0	-1.217912	-1.595552	1.529455
36	1	0	-1.613036	-0.659292	1.956071
37	1	0	-0.924714	-2.242664	2.363680
38	1	0	-2.035473	-2.095588	0.992032

Zero-point correction= 0.304809
(Hartree/Particle)
Thermal correction to Energy= 0.323776
Thermal correction to Enthalpy= 0.324721
Thermal correction to Gibbs Free Energy= 0.257679
Sum of electronic and zero-point Energies= -990.913971
Sum of electronic and thermal Energies= -990.895003
Sum of electronic and thermal Enthalpies= -990.894058
Sum of electronic and thermal Free Energies= -990.961100

It



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.762861	0.580729	-0.292311
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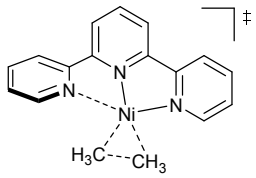
3	7	0	2.122957	-0.680219	-0.205356
4	6	0	3.684525	1.127395	-0.221155
5	6	0	4.464051	-1.140823	-0.274874
6	6	0	3.132450	-1.545166	-0.245360
7	6	0	2.378755	0.636557	-0.187538
8	1	0	3.880737	2.193333	-0.218116
9	1	0	5.258549	-1.877647	-0.307579
10	1	0	2.845402	-2.592956	-0.253225
11	6	0	1.177398	1.515061	-0.122658
12	6	0	-1.179658	2.918807	0.031676
13	6	0	1.226342	2.902748	0.018927
14	7	0	0.009504	0.871360	-0.188025
15	6	0	-1.149329	1.531211	-0.111548
16	6	0	0.028394	3.604336	0.093252

17	1	0	2.171399	3.428620	0.083944
18	1	0	0.036365	4.683075	0.209804
19	1	0	-2.117987	3.455348	0.107793
20	6	0	-2.362467	0.668771	-0.170323
21	6	0	-4.462547	-1.091430	-0.265919
22	6	0	-3.662753	1.171649	-0.226239
23	7	0	-2.120880	-0.649956	-0.167791
24	6	0	-3.135531	-1.508501	-0.214207
25	6	0	-4.724042	0.274792	-0.273138
26	1	0	-3.848855	2.239373	-0.241487
27	1	0	-2.854252	-2.558414	-0.211706
28	1	0	-5.744496	0.641701	-0.318657
29	1	0	-5.263871	-1.820546	-0.303414
30	28	0	-0.010662	-1.269164	0.148096
31	6	0	0.043178	-0.805289	2.171240
32	1	0	-0.848476	-0.239914	2.482511
33	1	0	0.924557	-0.201847	2.437161
34	1	0	0.077609	-1.727237	2.764747
35	6	0	-0.124683	-3.237640	-0.471445
36	1	0	-0.590993	-3.349213	-1.463394
37	1	0	-0.745151	-3.808002	0.236192
38	1	0	0.837260	-3.767775	-0.524783

Zero-point correction= 0.301958
(Hartree/Particle)
Thermal correction to Energy= 0.322138
Thermal correction to Enthalpy= 0.323082
Thermal correction to Gibbs Free Energy= 0.251593
Sum of electronic and zero-point Energies= -990.927518
Sum of electronic and thermal Energies= -990.907338
Sum of electronic and thermal Enthalpies= -990.906394
Sum of electronic and thermal Free Energies= -990.977883

TS-1s



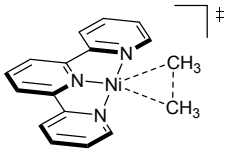
Imaginary frequency = -565.5764 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.670577	0.503666	0.340697
2	6	0	-4.646735	0.220424	0.119697
3	7	0	-2.002590	-0.530755	-0.428943
4	6	0	-3.620110	1.134453	0.250411
5	6	0	-4.337338	-1.087798	-0.286226
6	6	0	-3.018034	-1.409635	-0.533974
7	6	0	-2.304611	0.741542	-0.037959
8	1	0	-3.814232	2.145179	0.594902
9	1	0	-5.111584	-1.835733	-0.415152
10	1	0	-2.736405	-2.411414	-0.850000
11	6	0	-1.143917	1.614045	0.060251
12	6	0	1.252763	2.966599	-0.048049
13	6	0	-1.154043	2.998123	-0.068193
14	7	0	0.020742	0.926054	0.221950

15	6	0	1.204571	1.583682	0.080808
16	6	0	0.058602	3.688217	-0.094187
17	1	0	-2.094050	3.527158	-0.189067
18	1	0	0.073850	4.765394	-0.217615
19	1	0	2.207465	3.471891	-0.154011
20	6	0	2.345115	0.682773	-0.003183
21	6	0	4.349537	-1.174415	-0.270449
22	6	0	3.668818	1.056252	0.272972
23	7	0	2.019095	-0.588938	-0.378285
24	6	0	3.022734	-1.478457	-0.500544
25	6	0	4.681130	0.127681	0.135306
26	1	0	3.881023	2.066107	0.608923
27	1	0	2.727775	-2.474709	-0.818642
28	1	0	5.710964	0.397088	0.345590
29	1	0	5.111530	-1.932738	-0.410536
30	28	0	0.002167	-1.014580	-0.047408
31	6	0	-0.041222	-2.994836	-0.277307
32	1	0	0.906943	-3.517338	-0.153163
33	1	0	-0.132733	-2.677493	-1.336550
34	1	0	-0.858222	-3.689902	-0.079197
35	6	0	-0.252135	-2.274936	1.589466
36	1	0	0.256745	-1.471868	2.132785
37	1	0	0.155782	-3.227126	1.921563
38	1	0	-1.326439	-2.236733	1.770805

Zero-point correction= 0.303933
(Hartree/Particle)
Thermal correction to Energy= 0.322372
Thermal correction to Enthalpy= 0.323316
Thermal correction to Gibbs Free Energy= 0.257649
Sum of electronic and zero-point Energies= -990.861637
Sum of electronic and thermal Energies= -990.843198
Sum of electronic and thermal Enthalpies= -990.842254
Sum of electronic and thermal Free Energies= -990.907921

TS-1t



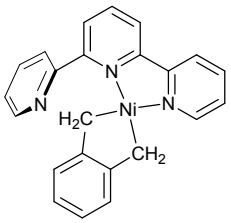
Imaginary frequency = -227.0953 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.767550	0.712561	-0.005203
2	6	0	-4.746550	0.343883	-0.004131
3	7	0	-2.129546	-0.598380	-0.005160
4	6	0	-3.690806	1.230065	-0.011567
5	6	0	-4.487711	-1.037305	0.006903
6	6	0	-3.166297	-1.443260	0.005775
7	6	0	-2.368586	0.741386	-0.009467
8	1	0	-3.876932	2.298068	-0.017566
9	1	0	-5.289179	-1.766483	0.016238
10	1	0	-2.905399	-2.499947	0.016107
11	6	0	-1.182873	1.584152	-0.006524
12	6	0	1.210942	2.969497	0.008370
13	6	0	-1.199286	2.977477	-0.007165

14	7	0	0.003269	0.899568	0.000517
15	6	0	1.179491	1.586438	0.007442
16	6	0	0.000450	3.681405	0.000694
17	1	0	-2.140260	3.517003	-0.013226
18	1	0	0.002277	4.765359	0.000790
19	1	0	2.152743	3.506461	0.014277
20	6	0	2.376668	0.734108	0.009232
21	6	0	4.492473	-1.038379	-0.009392
22	6	0	3.692011	1.225677	0.010238
23	7	0	2.136991	-0.598224	0.004454
24	6	0	3.169553	-1.446287	-0.007487
25	6	0	4.751286	0.337730	0.001786
26	1	0	3.876527	2.293595	0.016135
27	1	0	2.906967	-2.502148	-0.017931
28	1	0	5.772053	0.706803	0.002088
29	1	0	5.294008	-1.767744	-0.019554
30	28	0	-0.009045	-1.114489	0.000740
31	6	0	0.020198	-2.750596	-1.128872
32	1	0	0.753428	-3.546724	-1.011054
33	1	0	0.297593	-2.116390	-1.984120
34	1	0	-0.977130	-3.163348	-1.277149
35	6	0	-0.023929	-2.750259	1.131157
36	1	0	-0.298977	-2.116555	1.987341
37	1	0	0.973702	-3.164029	1.276021
38	1	0	-0.757814	-3.545931	1.015452

Zero-point correction=	0.301152
(Hartree/Particle)	
Thermal correction to Energy=	0.320276
Thermal correction to Enthalpy=	0.321220
Thermal correction to Gibbs Free Energy=	0.253070
Sum of electronic and zero-point Energies=	-990.915516
Sum of electronic and thermal Energies=	-990.896392
Sum of electronic and thermal Enthalpies=	-990.895448
Sum of electronic and thermal Free Energies=	-990.963598

IIs



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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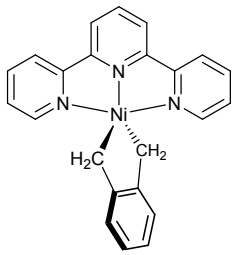
2	7	0	-1.333120	-0.993531	0.164564
3	6	0	-2.931329	-2.619852	1.747913
4	6	0	-0.962471	-2.252168	0.427002
5	6	0	-2.531467	-0.563061	0.592715
6	6	0	-3.356096	-1.343499	1.401757
7	6	0	-1.731729	-3.092951	1.234893
8	1	0	-4.302153	-0.961812	1.765959
9	1	0	-1.397905	-4.107397	1.423786
10	1	0	-3.545776	-3.248036	2.384600
11	7	0	0.355471	-2.470735	-1.550088
12	6	0	2.340173	-3.940138	-0.242062
13	6	0	1.434323	-2.903231	-2.197395

14	6	0	0.261483	-2.759714	-0.249574
15	6	0	1.214512	-3.502740	0.446083
16	6	0	2.457445	-3.632335	-1.592005
17	1	0	1.487486	-2.650967	-3.253526
18	1	0	1.093942	-3.692194	1.508033
19	1	0	3.321372	-3.943196	-2.168908
20	1	0	3.117768	-4.497111	0.270758
21	7	0	-1.938440	1.472555	-0.504200
22	6	0	-4.491650	2.538178	-0.353266
23	6	0	-2.920950	0.786302	0.102043
24	6	0	-2.205739	2.664991	-1.036260
25	6	0	-3.473224	3.236361	-0.990638
26	6	0	-4.215458	1.293963	0.201240
27	1	0	-1.365726	3.171105	-1.500363
28	1	0	-3.647052	4.205852	-1.442740
29	1	0	-5.000772	0.724849	0.684203
30	1	0	-5.493145	2.951709	-0.292240
31	6	0	0.856813	2.354426	-0.477421
32	1	0	0.292905	3.162907	0.016697
33	1	0	0.870531	2.595124	-1.555937
34	6	0	1.657451	-0.081675	0.291209
35	1	0	1.543641	-0.674797	1.215681
36	1	0	2.031903	-0.780627	-0.472256
37	6	0	2.667050	1.019977	0.490675
38	6	0	4.395611	3.207008	0.743883
39	6	0	2.257748	2.287941	0.070962
40	6	0	3.943815	0.855574	1.036695
41	6	0	4.804898	1.942258	1.166981
42	6	0	3.126025	3.375523	0.196427
43	1	0	4.260535	-0.132568	1.366768
44	1	0	5.792676	1.807093	1.599885
45	1	0	2.800335	4.361936	-0.129630
46	1	0	5.064125	4.057842	0.845332

Zero-point correction=	0.367243
(Hartree/Particle)	
Thermal correction to Energy=	0.389126
Thermal correction to Enthalpy=	0.390070
Thermal correction to Gibbs Free Energy=	0.315622
Sum of electronic and zero-point Energies=	-1220.620670
Sum of electronic and thermal Energies=	-1220.598787
Sum of electronic and thermal Enthalpies=	-1220.597843
Sum of electronic and thermal Free Energies=	-1220.672291

IIt

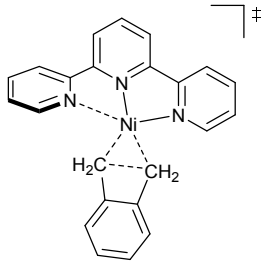


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.159677	-0.639380	-0.385103
2	7	0	1.284050	1.168551	-0.121338
3	6	0	2.687041	3.451170	0.487450

4	6	0	0.638253	2.336345	-0.060603
5	6	0	2.596899	1.090003	0.118578
6	6	0	3.341370	2.225559	0.435668
7	6	0	1.322313	3.517356	0.237514
8	1	0	4.404135	2.164942	0.636060
9	1	0	0.807670	4.469765	0.268753
10	1	0	3.241297	4.353727	0.723106
11	7	0	-1.290448	1.062202	-0.693976
12	6	0	-3.035474	3.195600	-0.358634
13	6	0	-2.598663	0.907091	-0.898909
14	6	0	-0.827077	2.264968	-0.315904
15	6	0	-1.670734	3.359863	-0.141105
16	6	0	-3.510365	1.949534	-0.741191
17	1	0	-2.924816	-0.090483	-1.177682
18	1	0	-1.283031	4.319714	0.179374
19	1	0	-4.565865	1.764399	-0.903419
20	1	0	-3.714422	4.030750	-0.218389
21	7	0	2.289931	-1.247840	-0.272799
22	6	0	4.955224	-1.879297	0.118454
23	6	0	3.171268	-0.281348	0.023859
24	6	0	2.705498	-2.507640	-0.378999
25	6	0	4.034645	-2.874390	-0.189528
26	6	0	4.522399	-0.562687	0.226607
27	1	0	1.934753	-3.232992	-0.623156
28	1	0	4.332884	-3.912292	-0.282147
29	1	0	5.227966	0.224866	0.463908
30	1	0	6.001652	-2.121985	0.273298
31	6	0	-0.813758	-2.417936	-0.891501
32	1	0	-0.203543	-3.183437	-0.384341
33	1	0	-1.015698	-2.772670	-1.908517
34	6	0	-0.591372	-1.064681	1.522490
35	1	0	0.021709	-1.929888	1.809669
36	1	0	-0.589668	-0.331253	2.336474
37	6	0	-1.960534	-1.452404	1.094297
38	6	0	-4.505843	-2.016320	0.020801
39	6	0	-2.074557	-2.177746	-0.129893
40	6	0	-3.126385	-1.008748	1.722555
41	6	0	-4.392620	-1.273663	1.191372
42	6	0	-3.349446	-2.469208	-0.623110
43	1	0	-3.038717	-0.425847	2.637948
44	1	0	-5.281876	-0.907391	1.697928
45	1	0	-3.434059	-3.025902	-1.554894
46	1	0	-5.484534	-2.240299	-0.395893

Zero-point correction=	0.365686
(Hartree/Particle)	
Thermal correction to Energy=	0.387660
Thermal correction to Enthalpy=	0.388604
Thermal correction to Gibbs Free Energy=	0.313130
Sum of electronic and zero-point Energies=	-1220.636472
Sum of electronic and thermal Energies=	-1220.614499
Sum of electronic and thermal Enthalpies=	-1220.613555
Sum of electronic and thermal Free Energies=	-1220.689029

TS-(II-IV)s



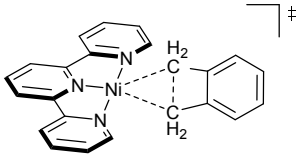
Imaginary frequency = -477.4416 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.165287	-0.183613	-0.233699
2	7	0	-1.771240	0.692223	0.300413
3	6	0	-4.226011	2.019281	0.168967
4	6	0	-2.943270	-0.018461	0.183447
5	6	0	-1.819688	2.061329	0.169919
6	6	0	-3.027290	2.740278	0.143356
7	6	0	-4.173920	0.625059	0.154210
8	1	0	-3.037432	3.822531	0.057901
9	1	0	-5.086526	0.042134	0.076088
10	1	0	-5.178315	2.534766	0.121745
11	7	0	-1.454813	-1.764297	-0.381514
12	6	0	-3.366697	-3.752320	0.172484
13	6	0	-1.163674	-3.079525	-0.485212
14	6	0	-2.721741	-1.434303	0.036332
15	6	0	-3.683087	-2.422196	0.321597
16	6	0	-2.063428	-4.092059	-0.240940
17	1	0	-0.150833	-3.317005	-0.797607
18	1	0	-4.660367	-2.118544	0.682228
19	1	0	-1.764524	-5.125004	-0.376889
20	1	0	-4.098575	-4.523864	0.387585
21	7	0	0.440241	1.756904	-0.424071
22	6	0	1.106163	4.428749	0.093740
23	6	0	-0.509685	2.647450	0.004402
24	6	0	1.705553	2.204711	-0.565337
25	6	0	2.081035	3.511362	-0.338589
26	6	0	-0.186708	3.987939	0.275157
27	1	0	2.437679	1.468232	-0.887986
28	1	0	3.109884	3.813001	-0.497469
29	1	0	-0.956886	4.655730	0.646937
30	1	0	1.370716	5.460754	0.299809
31	6	0	1.586311	-1.067971	-1.008995
32	1	0	1.370952	-0.312684	-1.777561
33	1	0	1.249439	-2.040153	-1.375673
34	6	0	1.401882	-1.109471	0.997628
35	1	0	1.021307	-0.330205	1.664417
36	1	0	0.949924	-2.073454	1.244748
37	6	0	2.890288	-1.128832	0.820910
38	6	0	5.382758	-1.119817	-0.342004
39	6	0	3.019688	-1.087048	-0.553053
40	6	0	3.994045	-1.176251	1.659442
41	6	0	5.251945	-1.168289	1.048063
42	6	0	4.259727	-1.080496	-1.175011
43	1	0	3.898570	-1.205704	2.740971
44	1	0	6.146182	-1.192186	1.663417

45	1	0	4.366292	-1.037970	-2.255441
46	1	0	6.376071	-1.107732	-0.780530

Zero-point correction= 0.364585
(Hartree/Particle)
Thermal correction to Energy= 0.386064
Thermal correction to Enthalpy= 0.387008
Thermal correction to Gibbs Free Energy= 0.313303
Sum of electronic and zero-point Energies= -1220.550444
Sum of electronic and thermal Energies= -1220.528964
Sum of electronic and thermal Enthalpies= -1220.528020
Sum of electronic and thermal Free Energies= -1220.601725

TS-(II-IV)t



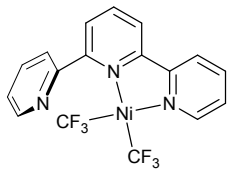
Imaginary frequency = -339.9511 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.080201	-0.324681	0.000522
2	7	0	-1.727697	0.827658	-0.000014
3	6	0	-4.033263	2.362638	-0.001014
4	6	0	-1.642878	2.173198	-0.000258
5	6	0	-2.950663	0.205025	-0.000299
6	6	0	-4.124024	0.989074	-0.000791
7	6	0	-2.759061	2.983076	-0.000760
8	1	0	-5.099237	0.513542	-0.000993
9	1	0	-2.679773	4.063288	-0.000971
10	1	0	-4.931556	2.970495	-0.001366
11	7	0	0.721657	1.754907	0.000371
12	6	0	1.395243	4.445324	0.000390
13	6	0	2.001894	2.139649	0.000678
14	6	0	-0.249703	2.690697	0.000061
15	6	0	0.065490	4.053823	0.000071
16	6	0	2.392498	3.470993	0.000697
17	1	0	2.736944	1.336737	0.000930
18	1	0	-0.722766	4.797186	-0.000156
19	1	0	3.444262	3.732909	0.000947
20	1	0	1.653022	5.499813	0.000402
21	7	0	-1.650527	-1.795057	0.000546
22	6	0	-3.917585	-3.426998	0.000045
23	6	0	-2.904303	-1.231223	-0.000020
24	6	0	-1.549079	-3.130279	0.000877
25	6	0	-2.625137	-3.995024	0.000670
26	6	0	-4.053448	-2.060830	-0.000296
27	1	0	-0.531322	-3.519889	0.001326
28	1	0	-2.472195	-5.067409	0.000959
29	1	0	-5.041594	-1.613806	-0.000810
30	1	0	-4.797877	-4.062358	-0.000180
31	6	0	1.433783	-1.294095	1.041806
32	1	0	1.026268	-2.268847	1.325154
33	1	0	1.151363	-0.545761	1.797455
34	6	0	1.433134	-1.294467	-1.041350
35	1	0	1.025331	-2.269223	-1.324271
36	1	0	1.150335	-0.546230	-1.796946

37	6	0	2.893896	-1.322762	-0.691640
38	6	0	5.270990	-1.368034	0.697318
39	6	0	2.894336	-1.322417	0.691201
40	6	0	4.073100	-1.349970	-1.422073
41	6	0	5.270537	-1.368433	-0.699293
42	6	0	4.074023	-1.349178	1.420876
43	1	0	4.077333	-1.344000	-2.508448
44	1	0	6.217311	-1.377377	-1.230834
45	1	0	4.078975	-1.342624	2.507245
46	1	0	6.218110	-1.376674	1.228250

Zero-point correction= 0.363188
(Hartree/Particle)
Thermal correction to Energy= 0.385218
Thermal correction to Enthalpy= 0.386162
Thermal correction to Gibbs Free Energy= 0.309368
Sum of electronic and zero-point Energies= -1220.608099
Sum of electronic and thermal Energies= -1220.586069
Sum of electronic and thermal Enthalpies= -1220.585124
Sum of electronic and thermal Free Energies= -1220.661919

IIIs

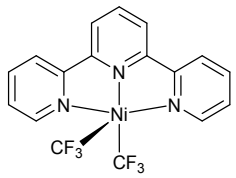


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.348446	-0.616742	0.029510
2	9	0	-1.462469	0.064139	1.949729
3	9	0	-2.253196	-1.554525	0.748403
4	9	0	1.770140	-2.893681	0.673580
5	9	0	1.218975	-2.673947	-1.411119
6	9	0	-0.230698	-3.390718	0.021016
7	9	0	-0.701905	-1.936850	2.200896
8	7	0	0.047139	1.390374	-0.047138
9	7	0	-2.050454	0.277925	-1.463377
10	7	0	2.249229	0.043453	-0.450084
11	6	0	1.169224	2.108247	0.097141
12	6	0	-3.552309	1.310642	0.106370
13	6	0	-1.259036	3.369878	0.134940
14	6	0	-4.588701	0.491928	-0.324751
15	6	0	-2.303913	1.161443	-0.493235
16	6	0	2.424126	1.329598	-0.085304
17	6	0	-0.108461	4.110249	0.370113
18	6	0	0.744039	-2.475992	-0.124770
19	6	0	-3.052429	-0.499587	-1.865548
20	6	0	1.131110	3.482551	0.323437
21	6	0	3.319170	-0.714236	-0.700766
22	6	0	-4.338122	-0.429824	-1.333787
23	6	0	3.692571	1.884557	0.055089
24	6	0	4.618507	-0.224692	-0.599813
25	6	0	4.805475	1.092617	-0.205473
26	6	0	-1.089271	-1.061739	1.239961
27	6	0	-1.142681	1.998276	-0.092410
28	1	0	-3.690541	2.016636	0.918615
29	1	0	-2.233440	3.842953	0.086997

30	1	0	-5.571228	0.564019	0.130634
31	1	0	-0.170732	5.179165	0.546797
32	1	0	-2.813593	-1.216529	-2.646577
33	1	0	2.041705	4.056346	0.443674
34	1	0	3.114550	-1.738454	-0.984907
35	1	0	-5.114215	-1.095002	-1.695549
36	1	0	3.815672	2.914555	0.367305
37	1	0	5.456842	-0.875370	-0.818897
38	1	0	5.803691	1.504926	-0.099892

Zero-point correction= 0.261394
(Hartree/Particle)
Thermal correction to Energy= 0.284425
Thermal correction to Enthalpy= 0.285369
Thermal correction to Gibbs Free Energy= 0.208389
Sum of electronic and zero-point Energies= -1586.276594
Sum of electronic and thermal Energies= -1586.253564
Sum of electronic and thermal Enthalpies= -1586.252620
Sum of electronic and thermal Free Energies= -1586.329599

IIIt

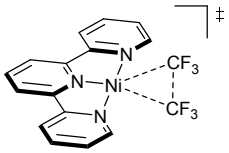


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.046032	-0.656007	-0.216160
2	9	0	-0.957007	0.653878	2.143991
3	9	0	-0.996848	-1.502782	2.332991
4	9	0	1.091297	-3.288524	0.294594
5	9	0	0.968482	-2.821896	-1.810267
6	9	0	-0.806105	-3.463307	-0.735844
7	9	0	0.870592	-0.429432	2.577637
8	7	0	-0.037102	1.423638	-0.443827
9	7	0	-2.055518	-0.237212	-0.537654
10	7	0	2.118612	-0.051102	-0.305737
11	6	0	1.097565	2.114681	-0.341465
12	6	0	-3.715018	1.471134	-0.422763
13	6	0	-1.337150	3.397022	-0.328544
14	6	0	-4.712194	0.500184	-0.435441
15	6	0	-2.385622	1.063099	-0.468652
16	6	0	2.331595	1.274907	-0.316879
17	6	0	-0.164979	4.140793	-0.241906
18	6	0	0.290192	-2.645689	-0.617295
19	6	0	-3.005302	-1.169406	-0.539508
20	6	0	1.072769	3.505336	-0.240415
21	6	0	3.147536	-0.893889	-0.264252
22	6	0	-4.358345	-0.841645	-0.491456
23	6	0	3.618983	1.803097	-0.298360
24	6	0	4.465542	-0.443507	-0.237881
25	6	0	4.699116	0.925568	-0.258443
26	6	0	-0.253461	-0.491467	1.806487
27	6	0	-1.233304	2.009263	-0.420519
28	1	0	-3.975365	2.521758	-0.367278
29	1	0	-2.300841	3.891485	-0.310522
30	1	0	-5.756038	0.794636	-0.396039

31	1	0	-0.216740	5.221793	-0.162357
32	1	0	-2.649447	-2.195241	-0.576288
33	1	0	1.985939	4.080958	-0.148179
34	1	0	2.890520	-1.948952	-0.245825
35	1	0	-5.107551	-1.624820	-0.493256
36	1	0	3.783356	2.874190	-0.317018
37	1	0	5.281283	-1.156042	-0.201639
38	1	0	5.712796	1.312853	-0.242774

Zero-point correction= 0.259644
(Hartree/Particle)
Thermal correction to Energy= 0.283602
Thermal correction to Enthalpy= 0.284546
Thermal correction to Gibbs Free Energy= 0.202237
Sum of electronic and zero-point Energies= -1586.285768
Sum of electronic and thermal Energies= -1586.261809
Sum of electronic and thermal Enthalpies= -1586.260865
Sum of electronic and thermal Free Energies= -1586.343175

TS-(III-IV)t



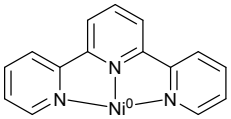
Imaginary frequency = -270.8174 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.019151	-0.306852	0.016016
2	9	0	0.768286	-1.577182	-1.913582
3	9	0	0.519192	-3.491371	-1.040178
4	9	0	-1.020716	-3.292132	0.862974
5	9	0	-0.540078	-1.536809	1.957683
6	9	0	1.057399	-2.803283	1.272905
7	9	0	-1.228181	-2.301844	-1.486852
8	7	0	0.035018	1.673271	-0.007160
9	7	0	2.104841	0.074873	0.086387
10	7	0	-2.100994	0.169435	0.009574
11	6	0	-1.118771	2.366118	-0.050732
12	6	0	3.725324	1.869639	0.080768
13	6	0	1.283686	3.711972	-0.034459
14	6	0	4.756189	0.961756	0.102274
15	6	0	2.383506	1.422291	0.063805
16	6	0	-2.325116	1.504395	-0.024616
17	6	0	0.103551	4.426221	-0.090428
18	6	0	-0.122382	-2.305246	0.932231
19	6	0	3.131778	-0.788848	0.096935
20	6	0	-1.137401	3.744744	-0.096404
21	6	0	-3.149514	-0.659311	0.079493
22	6	0	4.459941	-0.416827	0.104832
23	6	0	-3.626830	2.016118	-0.012942
24	6	0	-4.465198	-0.225360	0.102810
25	6	0	-4.704403	1.148041	0.048532
26	6	0	0.020782	-2.256553	-1.036198
27	6	0	1.246995	2.305959	0.008839
28	1	0	3.936353	2.933363	0.072224
29	1	0	2.231807	4.239232	-0.025881
30	1	0	5.786083	1.304628	0.113407

31	1	0	0.124120	5.509899	-0.127454
32	1	0	2.857762	-1.840717	0.098813
33	1	0	-2.064546	4.303887	-0.135302
34	1	0	-2.914400	-1.718714	0.116884
35	1	0	5.240245	-1.168200	0.114456
36	1	0	-3.788281	3.086944	-0.044496
37	1	0	-5.274926	-0.943216	0.161731
38	1	0	-5.718453	1.534636	0.060567

Zero-point correction= 0.258277
(Hartree/Particle)
Thermal correction to Energy= 0.280767
Thermal correction to Enthalpy= 0.281711
Thermal correction to Gibbs Free Energy= 0.204454
Sum of electronic and zero-point Energies= -1586.214858
Sum of electronic and thermal Energies= -1586.192368
Sum of electronic and thermal Enthalpies= -1586.191424
Sum of electronic and thermal Free Energies= -1586.268681

IVs

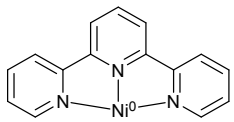


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.055464	-0.258751	-5.679816
2	6	0	0.216194	-0.155738	-4.634244
3	7	0	0.925894	0.136841	-1.948858
4	6	0	-0.750663	-0.208003	-3.653013
5	6	0	1.561136	0.008998	-4.259806
6	6	0	1.858423	0.150630	-2.920540
7	6	0	-0.382109	-0.078095	-2.304064
8	1	0	-1.792260	-0.380114	-3.903261
9	1	0	2.353240	0.047344	-4.998297
10	1	0	2.878308	0.314494	-2.585100
11	6	0	-1.295723	-0.148842	-1.182054
12	6	0	-2.641032	0.185884	1.203401
13	6	0	-2.641032	0.185884	-1.203401
14	7	0	-0.658427	-0.472096	0.000000
15	6	0	-1.295723	-0.148842	1.182054
16	6	0	-3.344600	0.299740	0.000000
17	1	0	-3.128298	0.410968	-2.147378
18	1	0	-4.391822	0.578680	0.000000
19	1	0	-3.128298	0.410968	2.147378
20	6	0	-0.382109	-0.078095	2.304064
21	6	0	1.561136	0.008998	4.259806
22	6	0	-0.750663	-0.208003	3.653013
23	7	0	0.925894	0.136841	1.948858
24	6	0	1.858423	0.150630	2.920540
25	6	0	0.216194	-0.155738	4.634244
26	1	0	-1.792260	-0.380114	3.903261
27	1	0	2.878308	0.314494	2.585100
28	1	0	-0.055464	-0.258751	5.679816
29	1	0	2.353240	0.047344	4.998297
30	28	0	1.171433	0.060211	-0.000000

Zero-point correction= 0.229752
(Hartree/Particle)

Thermal correction to Energy= 0.243869
Thermal correction to Enthalpy= 0.244813
Thermal correction to Gibbs Free Energy= 0.188635
Sum of electronic and zero-point Energies= -911.225343
Sum of electronic and thermal Energies= -911.211226
Sum of electronic and thermal Enthalpies= -911.210282
Sum of electronic and thermal Free Energies= -911.266460

IVt



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000053	0.246610	5.734017
2	6	0	0.000030	-0.092343	4.703062
3	7	0	-0.000022	-0.963824	2.045832
4	6	0	0.000057	0.820443	3.669324
5	6	0	-0.000022	-1.463675	4.399784
6	6	0	-0.000045	-1.833155	3.068938
7	6	0	0.000027	0.378366	2.335434
8	1	0	0.000107	1.884588	3.878478
9	1	0	-0.000040	-2.219112	5.176667
10	1	0	-0.000083	-2.883501	2.789484
11	6	0	0.000057	1.284442	1.187576
12	6	0	-0.000001	2.674061	-1.215736
13	6	0	-0.000001	2.674061	1.215736
14	7	0	0.000122	0.636769	-0.000000
15	6	0	0.000057	1.284442	-1.187576
16	6	0	-0.000014	3.370593	-0.000000
17	1	0	-0.000056	3.221894	2.152336
18	1	0	-0.000062	4.454903	-0.000000
19	1	0	-0.000056	3.221894	-2.152336
20	6	0	0.000027	0.378366	-2.335434
21	6	0	-0.000022	-1.463675	-4.399784
22	6	0	0.000057	0.820443	-3.669324
23	7	0	-0.000022	-0.963824	-2.045832
24	6	0	-0.000045	-1.833155	-3.068938
25	6	0	0.000030	-0.092343	-4.703062
26	1	0	0.000107	1.884588	-3.878478
27	1	0	-0.000083	-2.883501	-2.789484
28	1	0	0.000053	0.246610	-5.734017
29	1	0	-0.000040	-2.219112	-5.176667
30	28	0	-0.000057	-1.334320	0.000000

Zero-point correction= 0.226976
(Hartree/Particle)
Thermal correction to Energy= 0.241375
Thermal correction to Enthalpy= 0.242319
Thermal correction to Gibbs Free Energy= 0.184188
Sum of electronic and zero-point Energies= -911.280780
Sum of electronic and thermal Energies= -911.266381
Sum of electronic and thermal Enthalpies= -911.265437
Sum of electronic and thermal Free Energies= -911.323568

Ethane

$H_3C—CH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.019507	1.159380
2	6	0	0.000000	0.000000	0.763044
3	1	0	0.882919	-0.509753	1.159380
4	1	0	-0.882919	-0.509753	1.159380
5	6	0	-0.000000	-0.000000	-0.763044
6	1	0	0.882919	0.509753	-1.159380
7	1	0	-0.882919	0.509753	-1.159380
8	1	0	-0.000000	-1.019507	-1.159380

Zero-point correction= 0.075739
(Hartree/Particle)
Thermal correction to Energy= 0.079231
Thermal correction to Enthalpy= 0.080175
Thermal correction to Gibbs Free Energy= 0.054302
Sum of electronic and zero-point Energies= -79.695216
Sum of electronic and thermal Energies= -79.691724
Sum of electronic and thermal Enthalpies= -79.690780
Sum of electronic and thermal Free Energies= -79.716653

Benzocyclobutane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.522226	-0.733401
2	6	0	0.000000	1.436420	-0.717749
3	6	0	-0.000000	-1.436420	-0.717749
4	6	0	0.000000	0.695320	0.452344
5	6	0	0.000000	0.699472	-1.907970
6	6	0	-0.000000	-0.699472	-1.907970
7	6	0	-0.000000	-0.695320	0.452344
8	1	0	0.000000	1.223787	-2.859119
9	1	0	-0.000000	-1.223787	-2.859119
10	1	0	-0.000000	-2.522226	-0.733401
11	6	0	0.000000	0.785891	1.967897
12	1	0	-0.889857	1.240360	2.412694
13	1	0	0.889857	1.240360	2.412694
14	6	0	-0.000000	-0.785891	1.967897
15	1	0	-0.889857	-1.240360	2.412694
16	1	0	0.889857	-1.240360	2.412694

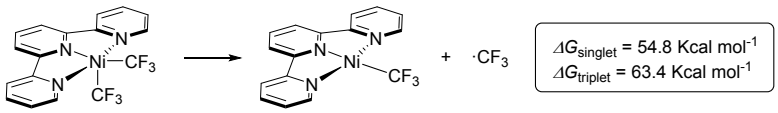
Zero-point correction= 0.136202
(Hartree/Particle)
Thermal correction to Energy= 0.142181
Thermal correction to Enthalpy= 0.143125
Thermal correction to Gibbs Free Energy= 0.106977
Sum of electronic and zero-point Energies= -309.346322
Sum of electronic and thermal Energies= -309.340343
Sum of electronic and thermal Enthalpies= -309.339399
Sum of electronic and thermal Free Energies= -309.375547

Hexafluoroethane

$CF_3—CF_3$

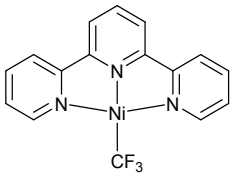
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.765543
2	6	0	-0.000000	-0.000000	-0.765543
3	9	0	1.083323	0.625457	-1.212162
4	9	0	-1.083323	0.625457	-1.212162
5	9	0	0.000000	1.250914	1.212162
6	9	0	1.083323	-0.625457	1.212162
7	9	0	-0.000000	-1.250914	-1.212162
8	9	0	-1.083323	-0.625457	1.212162

Zero-point correction= 0.030776
(Hartree/Particle)
Thermal correction to Energy= 0.037466
Thermal correction to Enthalpy= 0.038410
Thermal correction to Gibbs Free Energy= 0.000680
Sum of electronic and zero-point Energies= -675.007663
Sum of electronic and thermal Energies= -675.000973
Sum of electronic and thermal Enthalpies= -675.000029
Sum of electronic and thermal Free Energies= -675.037759



IIIs or **IIIt**

TPY-Ni-CF_3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.774034	0.488471	-0.000407
2	6	0	-4.716294	0.245511	-0.000370
3	7	0	-1.990025	-0.399527	-0.000184
4	6	0	-3.774469	1.245182	-0.000036
5	6	0	-4.288254	-1.096230	-0.000719
6	6	0	-2.934362	-1.359813	-0.000600
7	6	0	-2.402258	0.920701	0.000010
8	1	0	-4.071843	2.288428	0.000157
9	1	0	-4.994058	-1.917624	-0.001079
10	1	0	-2.563333	-2.374619	-0.000855
11	6	0	-1.341271	1.878707	0.000147
12	6	0	1.003107	3.391781	0.000307
13	6	0	-1.422421	3.280516	0.000358
14	7	0	-0.106379	1.289396	0.000035

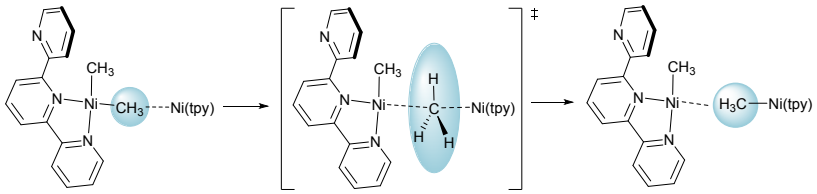
15	6	0	1.032724	2.015953	0.000101
16	6	0	-0.262449	4.031506	0.000438
17	1	0	-2.389849	3.771977	0.000445
18	1	0	-0.316926	5.114255	0.000609
19	1	0	1.914647	3.977701	0.000367
20	6	0	2.224134	1.155184	-0.000083
21	6	0	4.307897	-0.629849	-0.000624
22	6	0	3.533414	1.634595	-0.000152
23	7	0	1.956914	-0.180608	-0.000251
24	6	0	2.984546	-1.042977	-0.000530
25	6	0	4.587415	0.735447	-0.000413
26	1	0	3.713182	2.703362	-0.000017
27	1	0	2.726225	-2.092154	-0.000704
28	1	0	5.612222	1.092267	-0.000481
29	1	0	5.098489	-1.370721	-0.000866
30	28	0	-0.016594	-0.600998	0.000009
31	6	0	0.220442	-2.531282	0.000451
32	9	0	0.970251	-2.918341	1.083221
33	9	0	-0.831319	-3.392396	0.001190
34	9	0	0.969396	-2.919019	-1.082671

Zero-point correction= (Hartree/Particle)	0.245683
Thermal correction to Energy=	0.264014
Thermal correction to Enthalpy=	0.264958
Thermal correction to Gibbs Free Energy=	0.197805
Sum of electronic and zero-point Energies=	-1248.786794
Sum of electronic and thermal Energies=	-1248.768463
Sum of electronic and thermal Enthalpies=	-1248.767519
Sum of electronic and thermal Free Energies=	-1248.834672

·CF_3

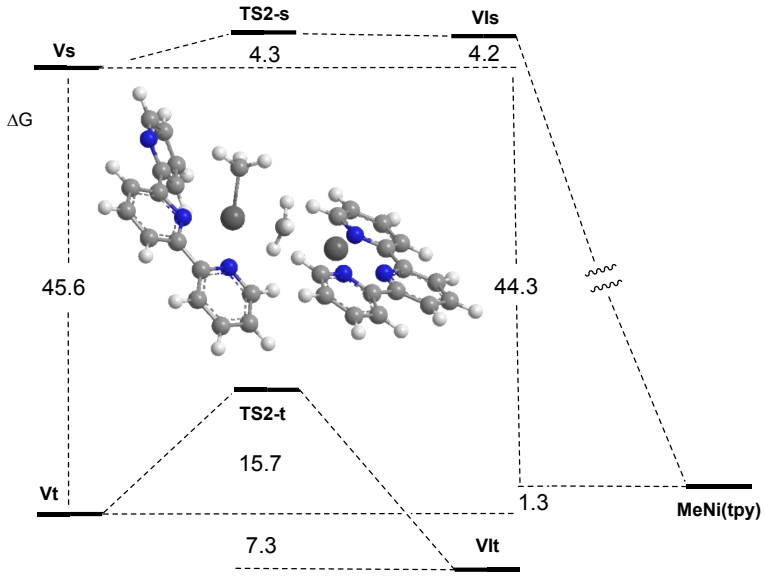
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	9	0	0.000000	1.311603	0.000000
3	9	0	1.135882	-0.655802	0.000000
4	9	0	-1.135882	-0.655802	0.000000

Zero-point correction= (Hartree/Particle)	0.011198
Thermal correction to Energy=	0.014570
Thermal correction to Enthalpy=	0.015514
Thermal correction to Gibbs Free Energy=	-0.013894
Sum of electronic and zero-point Energies=	-337.382456
Sum of electronic and thermal Energies=	-337.379084
Sum of electronic and thermal Enthalpies=	-337.378139
Sum of electronic and thermal Free Energies=	-337.407547

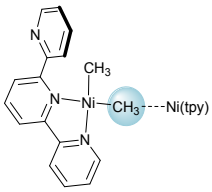


Vs or **Vt** **VIs** or **VIt**

	Vs	Vt
ΔG_a	4.3	15.7
ΔG	0.1	-7.3



Vs



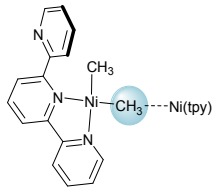
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.307686	-2.661403	-0.818672
2	6	0	-0.184936	-3.988960	-1.216543
3	6	0	-1.338017	-4.759568	-1.300805
4	7	0	-1.480986	-2.105765	-0.515748
5	6	0	-2.567162	-4.176974	-1.008410
6	6	0	-2.605152	-2.838734	-0.622465
7	6	0	-3.867195	-2.090616	-0.368328
8	7	0	-3.706655	-0.771181	-0.154396
9	6	0	-5.128741	-2.676664	-0.409360
10	6	0	-6.246570	-1.861839	-0.255084
11	6	0	-4.780809	0.026493	-0.107412
12	6	0	-6.078552	-0.491858	-0.131031
13	6	0	-4.564398	1.497516	-0.117606
14	6	0	-3.424666	2.041644	-0.714126
15	7	0	-5.544494	2.240183	0.404603
16	6	0	-3.285107	3.423143	-0.731329

17	6	0	-5.390592	3.562622	0.393245
18	6	0	-4.280741	4.203833	-0.154022
19	28	0	-1.813038	-0.405057	0.627070
20	6	0	0.068251	-0.258262	1.180608
21	6	0	-2.318142	0.867996	1.999436
22	1	0	0.567848	-2.023330	-0.736803
23	1	0	0.796961	-4.393332	-1.435941
24	1	0	-1.288026	-5.801827	-1.598920
25	1	0	-3.477969	-4.758312	-1.087130
26	1	0	-5.245314	-3.743771	-0.554240
27	1	0	-7.241668	-2.294919	-0.266320
28	1	0	-6.913138	0.194793	-0.059591
29	1	0	-2.672921	1.393121	-1.151069
30	1	0	-2.412251	3.876357	-1.191379
31	1	0	-6.196299	4.139459	0.840811
32	1	0	-4.211273	5.285879	-0.135545
33	1	0	0.291924	0.601395	1.814368
34	1	0	0.480093	-0.168567	0.152312
35	1	0	0.381178	-1.186166	1.666634
36	1	0	-1.874903	0.560916	2.953097
37	1	0	-3.409478	0.904870	2.125584
38	1	0	-1.968833	1.886349	1.783799
39	6	0	0.691350	2.744588	0.035331
40	6	0	0.560042	4.103214	-0.139128
41	6	0	1.715277	4.865040	-0.422101
42	7	0	1.872341	2.095936	-0.065655
43	6	0	2.929300	4.228031	-0.510368
44	6	0	3.004190	2.830901	-0.336291
45	6	0	4.203544	2.045930	-0.368452
46	7	0	4.050450	0.807182	0.248587
47	6	0	5.393654	2.393924	-0.973639
48	6	0	6.423947	1.443316	-1.088572
49	6	0	4.966408	-0.196254	-0.078545
50	6	0	6.172965	0.132903	-0.686873
51	6	0	4.495384	-1.497909	0.234438
52	6	0	5.302286	-2.656400	0.350672
53	7	0	3.130416	-1.563828	0.479403
54	6	0	4.747013	-3.855821	0.707206
55	6	0	2.627548	-2.750676	0.895069
56	6	0	3.359322	-3.906638	0.999856
57	28	0	2.296977	0.233437	0.450105
58	1	0	-0.172903	2.123934	0.263507
59	1	0	-0.412949	4.569649	-0.036599
60	1	0	1.648224	5.941063	-0.547592
61	1	0	3.842325	4.786483	-0.688427
62	1	0	5.508911	3.381372	-1.410874
63	1	0	7.353124	1.699031	-1.583953
64	1	0	6.897828	-0.649049	-0.895008
65	1	0	6.369399	-2.568678	0.173555
66	1	0	5.362386	-4.745543	0.794538
67	1	0	1.569502	-2.752624	1.139056
68	1	0	2.878371	-4.825998	1.313488

Zero-point correction=	0.536823
(Hartree/Particle)	
Thermal correction to Energy=	0.571349
Thermal correction to Enthalpy=	0.572293
Thermal correction to Gibbs Free Energy=	0.469557
Sum of electronic and zero-point Energies=	-1902.172727
Sum of electronic and thermal Energies=	-1902.138201
Sum of electronic and thermal Enthalpies=	-1902.137257

Sum of electronic and thermal Free Energies= -1902.239993

Vt

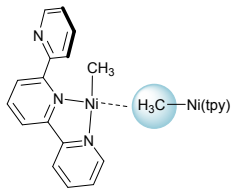


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827370	-0.048788	1.736654
2	6	0	-1.668765	-1.063042	2.186388
3	6	0	-1.200100	-2.368288	2.157002
4	7	0	0.409921	-0.278205	1.292978
5	6	0	0.091238	-2.615631	1.706365
6	6	0	0.872907	-1.540991	1.281147
7	6	0	2.282245	-1.695577	0.836166
8	7	0	2.928194	-0.546630	0.571368
9	6	0	2.918754	-2.933314	0.747269
10	6	0	4.263268	-2.968052	0.403189
11	6	0	4.245814	-0.574652	0.324784
12	6	0	4.947941	-1.775806	0.213314
13	6	0	4.981787	0.716118	0.250079
14	6	0	4.514221	1.845144	0.926338
15	7	0	6.128977	0.697415	-0.435890
16	6	0	5.260661	3.013897	0.852456
17	6	0	6.828874	1.827409	-0.504617
18	6	0	6.439524	3.012656	0.115146
19	28	0	1.534873	0.918786	0.010096
20	6	0	0.160105	2.236904	-0.446187
21	6	0	2.548709	1.611759	-1.509165
22	1	0	-1.156738	0.984672	1.723214
23	1	0	-2.678140	-0.828907	2.508322
24	1	0	-1.840104	-3.189838	2.463734
25	1	0	0.471962	-3.628330	1.671559
26	1	0	2.371394	-3.851222	0.921367
27	1	0	4.778176	-3.919065	0.309986
28	1	0	6.006083	-1.740431	-0.013766
29	1	0	3.582422	1.802094	1.479491
30	1	0	4.924301	3.912098	1.360971
31	1	0	7.749257	1.783653	-1.082114
32	1	0	7.050750	3.904028	0.025508
33	1	0	0.605387	3.219268	-0.642198
34	1	0	-0.608221	2.386359	0.328450
35	1	0	-0.324986	1.982667	-1.419724
36	1	0	1.892747	1.764616	-2.375317
37	1	0	3.344279	0.913509	-1.809822
38	1	0	3.016652	2.578090	-1.281758
39	6	0	-3.311543	3.474679	-0.244606
40	6	0	-4.387662	4.268046	0.135162
41	6	0	-5.565715	3.634057	0.518857
42	7	0	-3.357398	2.140891	-0.252701
43	6	0	-5.619232	2.246113	0.515727
44	6	0	-4.492763	1.518312	0.129074
45	6	0	-4.456945	0.025401	0.105246
46	7	0	-3.363169	-0.462841	-0.481786
47	6	0	-5.426883	-0.789266	0.663681
48	6	0	-5.223823	-2.192870	0.569314

49	6	0	-3.113620	-1.805630	-0.542716
50	6	0	-4.090247	-2.696478	-0.023614
51	6	0	-1.828887	-2.154407	-1.076211
52	6	0	-1.357417	-3.487868	-1.186260
53	7	0	-1.005464	-1.104651	-1.436780
54	6	0	-0.087928	-3.737557	-1.651062
55	6	0	0.216724	-1.378005	-1.908364
56	6	0	0.736032	-2.656046	-2.031275
57	28	0	-1.829543	0.771616	-0.955240
58	1	0	-2.364820	3.911105	-0.554961
59	1	0	-4.301195	5.348460	0.122662
60	1	0	-6.435298	4.213542	0.812565
61	1	0	-6.529581	1.728175	0.794347
62	1	0	-6.302229	-0.389489	1.160835
63	1	0	-5.967484	-2.870827	0.976275
64	1	0	-3.941691	-3.770342	-0.080722
65	1	0	-2.002550	-4.311738	-0.897182
66	1	0	0.270467	-4.759881	-1.735353
67	1	0	0.815274	-0.509782	-2.180972
68	1	0	1.737793	-2.804954	-2.417355

Zero-point correction=	0.535362
(Hartree/Particle)	
Thermal correction to Energy=	0.570495
Thermal correction to Enthalpy=	0.571439
Thermal correction to Gibbs Free Energy=	0.466304
Sum of electronic and zero-point Energies=	-1902.243537
Sum of electronic and thermal Energies=	-1902.208403
Sum of electronic and thermal Enthalpies=	-1902.207459
Sum of electronic and thermal Free Energies=	-1902.312595

VIs

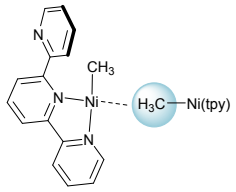


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101826	-2.218400	-0.930950
2	6	0	0.182241	-3.521648	-1.324791
3	6	0	-0.881967	-4.424909	-1.418222
4	7	0	-1.329515	-1.803254	-0.619695
5	6	0	-2.167170	-3.992798	-1.129491
6	6	0	-2.376244	-2.668574	-0.731447
7	6	0	-3.687725	-2.085579	-0.451931
8	7	0	-3.688046	-0.752244	-0.176054
9	6	0	-4.885745	-2.808788	-0.503714
10	6	0	-6.085284	-2.145483	-0.317777
11	6	0	-4.860864	-0.095126	-0.108162
12	6	0	-6.080833	-0.759660	-0.149308
13	6	0	-4.844635	1.392481	-0.093649
14	6	0	-3.849082	2.098201	-0.775180
15	7	0	-5.861604	1.990245	0.535058
16	6	0	-3.895280	3.485999	-0.763627
17	6	0	-5.887978	3.321236	0.544328
18	6	0	-4.929092	4.116572	-0.079331
19	28	0	-1.877183	-0.164601	0.480477

20	6	0	0.258065	0.396783	0.907603
21	6	0	-2.498224	1.033731	1.856880
22	1	0	0.695567	-1.486302	-0.829364
23	1	0	1.204481	-3.802808	-1.547773
24	1	0	-0.709077	-5.454061	-1.715289
25	1	0	-3.001476	-4.679465	-1.214895
26	1	0	-4.872305	-3.876066	-0.688411
27	1	0	-7.021807	-2.693058	-0.342430
28	1	0	-6.992207	-0.181059	-0.066735
29	1	0	-3.063009	1.562376	-1.296988
30	1	0	-3.136800	4.064172	-1.282491
31	1	0	-6.720057	3.777087	1.075703
32	1	0	-5.002723	5.197602	-0.035774
33	1	0	0.031065	1.188385	1.617211
34	1	0	-0.079590	0.628915	-0.116963
35	1	0	0.006356	-0.593081	1.301470
36	1	0	-1.939831	0.784049	2.766526
37	1	0	-3.566787	0.912590	2.061324
38	1	0	-2.301945	2.082800	1.605467
39	6	0	1.384081	3.247767	0.122598
40	6	0	1.572874	4.574689	-0.205657
41	6	0	2.845974	4.990006	-0.630593
42	7	0	2.360697	2.323429	0.055008
43	6	0	3.858515	4.054492	-0.707765
44	6	0	3.603341	2.721599	-0.367382
45	6	0	4.575760	1.641662	-0.418502
46	7	0	4.059900	0.471008	0.044116
47	6	0	5.863518	1.715696	-0.895505
48	6	0	6.640793	0.528114	-0.923622
49	6	0	4.773895	-0.713014	-0.023000
50	6	0	6.091504	-0.670184	-0.505418
51	6	0	4.020313	-1.823424	0.406511
52	6	0	4.476822	-3.161566	0.470786
53	7	0	2.705072	-1.506938	0.787677
54	6	0	3.655584	-4.162256	0.917130
55	6	0	1.945605	-2.511247	1.273605
56	6	0	2.339524	-3.826063	1.341748
57	28	0	2.256765	0.391278	0.527670
58	1	0	0.416488	2.889985	0.458168
59	1	0	0.747392	5.272248	-0.125995
60	1	0	3.032855	6.026439	-0.891309
61	1	0	4.855119	4.338847	-1.027169
62	1	0	6.273952	2.650977	-1.259708
63	1	0	7.658869	0.559668	-1.295099
64	1	0	6.677485	-1.583059	-0.555877
65	1	0	5.494225	-3.379595	0.159858
66	1	0	4.007098	-5.187755	0.962026
67	1	0	0.954230	-2.233866	1.617518
68	1	0	1.659861	-4.570495	1.739117

Zero-point correction= 0.536068
(Hartree/Particle)
Thermal correction to Energy= 0.570494
Thermal correction to Enthalpy= 0.571439
Thermal correction to Gibbs Free Energy= 0.469071
Sum of electronic and zero-point Energies= -1902.166276
Sum of electronic and thermal Energies= -1902.131850
Sum of electronic and thermal Enthalpies= -1902.130906
Sum of electronic and thermal Free Energies= -1902.233274

VIt

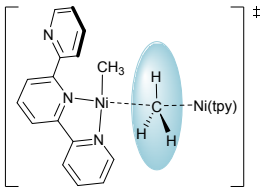


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.341010	-1.430532	2.258561
2	6	0	-2.583186	-0.953049	2.667708
3	6	0	-2.782089	0.423364	2.686414
4	7	0	-0.351270	-0.622991	1.885291
5	6	0	-1.743218	1.267180	2.308677
6	6	0	-0.529537	0.705377	1.909586
7	6	0	0.649024	1.510246	1.484964
8	7	0	1.671925	0.811354	0.963297
9	6	0	0.700778	2.893035	1.640674
10	6	0	1.845756	3.570056	1.232029
11	6	0	2.771505	1.462322	0.563663
12	6	0	2.896449	2.850676	0.687432
13	6	0	3.898972	0.667370	0.007825
14	6	0	3.667548	-0.505245	-0.713467
15	7	0	5.120986	1.162717	0.238684
16	6	0	4.768070	-1.221377	-1.169460
17	6	0	6.162786	0.466988	-0.210972
18	6	0	6.043131	-0.735617	-0.905297
19	28	0	1.489364	-1.328577	1.128035
20	6	0	1.188062	0.375056	-2.650703
21	6	0	2.197538	-3.257197	1.172266
22	1	0	-1.115074	-2.493508	2.213189
23	1	0	-3.368278	-1.643055	2.956589
24	1	0	-3.738322	0.839104	2.989322
25	1	0	-1.890731	2.341159	2.299490
26	1	0	-0.129129	3.435417	2.078630
27	1	0	1.913505	4.647813	1.344947
28	1	0	3.819200	3.319328	0.367869
29	1	0	2.650541	-0.805549	-0.947867
30	1	0	4.624748	-2.140977	-1.728098
31	1	0	7.143507	0.890455	-0.005701
32	1	0	6.930148	-1.264059	-1.237960
33	1	0	0.771006	0.864542	-3.549628
34	1	0	1.936036	1.082770	-2.248091
35	1	0	1.769813	-0.481105	-3.030148
36	1	0	1.426686	-3.992798	1.452871
37	1	0	3.009209	-3.358386	1.907858
38	1	0	2.610717	-3.595222	0.207169
39	6	0	-0.431137	3.138573	-1.381467
40	6	0	-0.934565	4.434327	-1.289263
41	6	0	-2.271198	4.597784	-0.939998
42	7	0	-1.179691	2.065593	-1.142163
43	6	0	-3.058151	3.474225	-0.707438
44	6	0	-2.472360	2.212610	-0.823721
45	6	0	-3.211594	0.933328	-0.619562
46	7	0	-2.465631	-0.169675	-0.753665
47	6	0	-4.572483	0.858955	-0.320168
48	6	0	-5.150729	-0.396991	-0.172519
49	6	0	-3.010082	-1.382543	-0.602234
50	6	0	-4.368289	-1.536161	-0.316193

51	6	0	-2.054992	-2.518093	-0.742244
52	6	0	-2.386397	-3.836805	-0.436466
53	7	0	-0.824682	-2.172488	-1.147435
54	6	0	-1.401562	-4.815317	-0.555129
55	6	0	0.113671	-3.107406	-1.257896
56	6	0	-0.128977	-4.451609	-0.972542
57	28	0	-0.455450	-0.013655	-1.431649
58	1	0	0.601772	2.927426	-1.650480
59	1	0	-0.293740	5.286243	-1.488061
60	1	0	-2.703453	5.590109	-0.856681
61	1	0	-4.104821	3.587033	-0.447758
62	1	0	-5.174275	1.754341	-0.216294
63	1	0	-6.209923	-0.486948	0.046770
64	1	0	-4.810611	-2.520383	-0.215980
65	1	0	-3.381818	-4.102761	-0.098400
66	1	0	-1.630005	-5.848744	-0.314042
67	1	0	1.088500	-2.756968	-1.582500
68	1	0	0.673304	-5.175543	-1.052221

Zero-point correction= (Hartree/Particle)	0.533165
Thermal correction to Energy=	0.569914
Thermal correction to Enthalpy=	0.570858
Thermal correction to Gibbs Free Energy=	0.460923
Sum of electronic and zero-point Energies=	-1902.251974
Sum of electronic and thermal Energies=	-1902.215226
Sum of electronic and thermal Enthalpies=	-1902.214282
Sum of electronic and thermal Free Energies=	-1902.324216

TS-2s



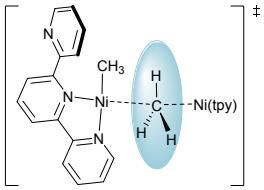
Imaginary frequency = -365.5809 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.157999	-2.286270	0.997456
2	6	0	-0.086178	-3.590578	1.415566
3	6	0	0.994390	-4.469314	1.488266
4	7	0	1.369902	-1.849477	0.652352
5	6	0	2.263655	-4.013922	1.156107
6	6	0	2.429165	-2.691864	0.740703
7	6	0	3.733067	-2.087928	0.416165
8	7	0	3.709077	-0.754712	0.171573
9	6	0	4.931001	-2.806031	0.401816
10	6	0	6.119440	-2.127988	0.177250
11	6	0	4.869705	-0.086462	0.058429
12	6	0	6.097260	-0.743697	0.034554
13	6	0	4.837401	1.400767	0.052381
14	6	0	3.835384	2.095051	0.735358
15	7	0	5.847821	2.008548	-0.577250
16	6	0	3.867351	3.483367	0.723059
17	6	0	5.861232	3.339519	-0.586360
18	6	0	4.894213	4.124345	0.038402
19	28	0	1.858762	-0.181254	-0.468252

20	6	0	-0.204501	0.273037	-0.836434
21	6	0	2.431784	1.024697	-1.864063
22	1	0	-0.659267	-1.574444	0.908640
23	1	0	-1.096635	-3.892748	1.663547
24	1	0	0.851785	-5.497310	1.804858
25	1	0	3.114567	-4.681281	1.225822
26	1	0	4.933006	-3.877529	0.560170
27	1	0	7.059676	-2.669029	0.148652
28	1	0	6.999515	-0.156673	-0.083242
29	1	0	3.053967	1.552043	1.256252
30	1	0	3.102143	4.053614	1.240766
31	1	0	6.688090	3.803967	-1.118214
32	1	0	4.956267	5.206071	-0.005327
33	1	0	-0.061965	1.097428	-1.522601
34	1	0	-0.059894	0.453441	0.232230
35	1	0	-0.146693	-0.728636	-1.248716
36	1	0	1.870352	0.771784	-2.770591
37	1	0	3.501138	0.917463	-2.079633
38	1	0	2.229002	2.073913	-1.616777
39	6	0	-1.243523	3.143066	0.057394
40	6	0	-1.380037	4.481479	0.355958
41	6	0	-2.663883	4.979357	0.651050
42	7	0	-2.275179	2.275928	0.046352
43	6	0	-3.732197	4.109568	0.642832
44	6	0	-3.527372	2.751194	0.354067
45	6	0	-4.552745	1.733645	0.331909
46	7	0	-4.107309	0.556139	-0.216712
47	6	0	-5.829673	1.849007	0.831870
48	6	0	-6.662286	0.704958	0.854305
49	6	0	-4.850974	-0.607080	-0.058366
50	6	0	-6.153119	-0.517942	0.444405
51	6	0	-4.134371	-1.769014	-0.416876
52	6	0	-4.680729	-3.070173	-0.537498
53	7	0	-2.779484	-1.542998	-0.688560
54	6	0	-3.897920	-4.125083	-0.921284
55	6	0	-2.057081	-2.597454	-1.130396
56	6	0	-2.532473	-3.881084	-1.236622
57	28	0	-2.273303	0.362477	-0.501598
58	1	0	-0.270154	2.725791	-0.183156
59	1	0	-0.509174	5.126418	0.353362
60	1	0	-2.811622	6.030620	0.875531
61	1	0	-4.737287	4.459933	0.852005
62	1	0	-6.180369	2.791088	1.240431
63	1	0	-7.667138	0.773475	1.254955
64	1	0	-6.753942	-1.417309	0.543815
65	1	0	-5.736605	-3.212839	-0.329185
66	1	0	-4.317400	-5.121737	-1.011252
67	1	0	-1.026239	-2.390741	-1.399978
68	1	0	-1.875696	-4.672064	-1.579263

Zero-point correction= 0.534947
(Hartree/Particle)
Thermal correction to Energy= 0.569100
Thermal correction to Enthalpy= 0.570044
Thermal correction to Gibbs Free Energy= 0.468627
Sum of electronic and zero-point Energies= -1902.166791
Sum of electronic and thermal Energies= -1902.132638
Sum of electronic and thermal Enthalpies= -1902.131694
Sum of electronic and thermal Free Energies= -1902.233111

TS-2t



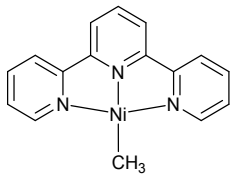
Imaginary frequency = -467.3528 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.473638	-2.113597	1.334751
2	6	0	0.281165	-3.401273	1.794252
3	6	0	1.385122	-4.289825	1.740619
4	7	0	1.626245	-1.654484	0.829527
5	6	0	2.585869	-3.839491	1.256547
6	6	0	2.720645	-2.499130	0.805702
7	6	0	3.937327	-1.921201	0.334921
8	7	0	3.908051	-0.562936	0.100258
9	6	0	5.129148	-2.657029	0.109583
10	6	0	6.270783	-2.007593	-0.282084
11	6	0	5.068791	0.067555	-0.190131
12	6	0	6.257649	-0.600618	-0.405236
13	6	0	5.074493	1.556005	-0.159203
14	6	0	4.232181	2.245545	0.721040
15	7	0	5.959852	2.179869	-0.944518
16	6	0	4.293720	3.630753	0.757151
17	6	0	6.001228	3.510156	-0.904288
18	6	0	5.190170	4.286589	-0.080832
19	28	0	2.011256	0.088021	-0.214435
20	6	0	-0.067857	0.695214	-0.216807
21	6	0	2.400665	1.322870	-1.695069
22	1	0	-0.352959	-1.403300	1.337395
23	1	0	-0.682750	-3.706696	2.184630
24	1	0	1.288701	-5.311103	2.097029
25	1	0	3.446115	-4.499762	1.241159
26	1	0	5.127981	-3.734395	0.233217
27	1	0	7.183421	-2.564893	-0.469670
28	1	0	7.147422	-0.031605	-0.641466
29	1	0	3.550798	1.688738	1.355308
30	1	0	3.652518	4.191994	1.430816
31	1	0	6.724535	3.982221	-1.566354
32	1	0	5.269619	5.368333	-0.093758
33	1	0	0.084777	1.666821	-0.669500
34	1	0	-0.033460	0.601564	0.866878
35	1	0	-0.021858	-0.181806	-0.862385
36	1	0	1.641778	1.177454	-2.475982
37	1	0	3.387752	1.132273	-2.133324
38	1	0	2.361319	2.373307	-1.377718
39	6	0	-2.274027	3.504244	0.390629
40	6	0	-2.828669	4.732515	0.742620
41	6	0	-4.206815	4.811402	0.899297
42	7	0	-3.011307	2.414598	0.194271
43	6	0	-4.979737	3.672295	0.697658
44	6	0	-4.343637	2.484709	0.340100
45	6	0	-5.075855	1.206311	0.098850
46	7	0	-4.292911	0.148324	-0.130336
47	6	0	-6.465439	1.087141	0.098349
48	6	0	-7.021155	-0.163635	-0.149868

49	6	0	-4.811668	-1.060137	-0.363409
50	6	0	-6.194524	-1.255407	-0.384242
51	6	0	-3.810885	-2.138853	-0.602171
52	6	0	-4.159222	-3.484805	-0.666635
53	7	0	-2.537204	-1.726140	-0.743313
54	6	0	-3.159115	-4.429551	-0.886456
55	6	0	-1.588137	-2.632636	-0.965586
56	6	0	-1.848860	-4.000702	-1.040795
57	28	0	-2.225151	0.416436	-0.260776
58	1	0	-1.203278	3.373083	0.259571
59	1	0	-2.191247	5.596682	0.890991
60	1	0	-4.679727	5.747580	1.178413
61	1	0	-6.055167	3.714613	0.825555
62	1	0	-7.105142	1.943684	0.273844
63	1	0	-8.099294	-0.285167	-0.167177
64	1	0	-6.621113	-2.229086	-0.593256
65	1	0	-5.186524	-3.802400	-0.529712
66	1	0	-3.406749	-5.485319	-0.928042
67	1	0	-0.576302	-2.252991	-1.076235
68	1	0	-1.033153	-4.696180	-1.201098

Zero-point correction= 0.533521
(Hartree/Particle)
Thermal correction to Energy= 0.568942
Thermal correction to Enthalpy= 0.569886
Thermal correction to Gibbs Free Energy= 0.462345
Sum of electronic and zero-point Energies= -1902.216460
Sum of electronic and thermal Energies= -1902.181039
Sum of electronic and thermal Enthalpies= -1902.180095
Sum of electronic and thermal Free Energies= -1902.287636

Ni(tpy)Me

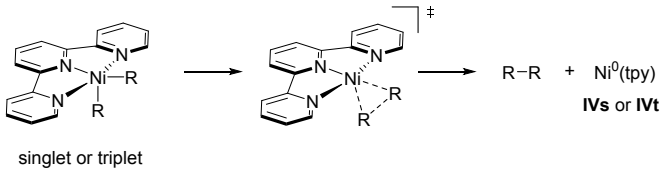


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.312454	0.062145	5.703468
2	6	0	0.018215	0.057040	4.658819
3	7	0	-0.744774	0.028314	1.979213
4	6	0	0.975693	-0.006913	3.667109
5	6	0	-1.335867	0.118943	4.299209
6	6	0	-1.661342	0.097193	2.955488
7	6	0	0.581598	-0.009049	2.320974
8	1	0	2.030349	-0.052761	3.915968
9	1	0	-2.118700	0.182246	5.045414
10	1	0	-2.692477	0.138408	2.622285
11	6	0	1.493719	-0.034774	1.189194
12	6	0	2.879839	-0.007420	-1.213722
13	6	0	2.879839	-0.007420	1.213722
14	7	0	0.832282	-0.070521	-0.000000
15	6	0	1.493719	-0.034774	-1.189194
16	6	0	3.580286	-0.002118	-0.000000
17	1	0	3.419298	0.018811	2.154860
18	1	0	4.663841	0.023117	-0.000000
19	1	0	3.419298	0.018811	-2.154860

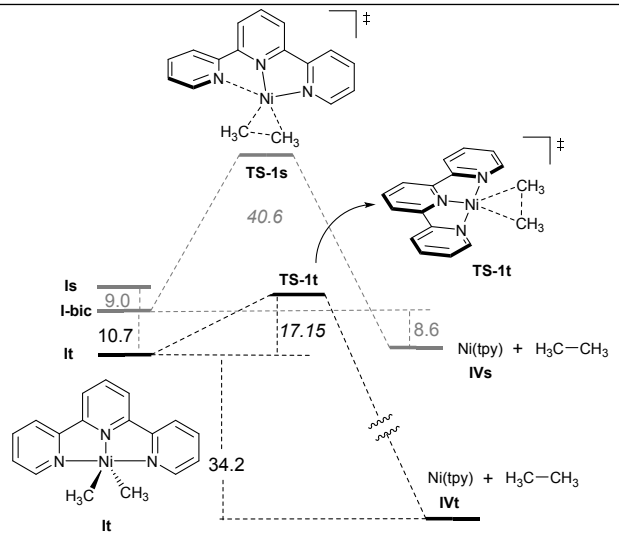
20	6	0	0.581598	-0.009049	-2.320974
21	6	0	-1.335867	0.118943	-4.299209
22	6	0	0.975693	-0.006913	-3.667109
23	7	0	-0.744774	0.028314	-1.979213
24	6	0	-1.661342	0.097193	-2.955488
25	6	0	0.018215	0.057040	-4.658819
26	1	0	2.030349	-0.052761	-3.915968
27	1	0	-2.692477	0.138408	-2.622285
28	1	0	0.312454	0.062145	-5.703468
29	1	0	-2.118700	0.182246	-5.045414
30	28	0	-1.084204	-0.050987	0.000000
31	6	0	-3.033058	-0.185607	0.000000
32	1	0	-3.406540	-0.730005	-0.876522
33	1	0	-3.499649	0.810185	0.000000
34	1	0	-3.406540	-0.730005	0.876522

Zero-point correction= 0.264657
(Hartree/Particle)
Thermal correction to Energy= 0.280213
Thermal correction to Enthalpy= 0.281157
Thermal correction to Gibbs Free Energy= 0.221558
Sum of electronic and zero-point Energies= -951.112169
Sum of electronic and thermal Energies= -951.096613
Sum of electronic and thermal Enthalpies= -951.095669
Sum of electronic and thermal Free Energies= -951.155268

I.3. Atomic coordinates and energies for the stationary points in THF



	I-bic R = CH_3 singlet	**It** R = CH_3 triplet	**IIs** singlet	**IIt** triplet	**IIIs** R = CF_3 singlet	**IIIt** R = CF_3 triplet
ΔG_a	40.6	17.1	52.2	24.4	-	58.6
ΔG	-8.9	-34.1	24.3	-1,7	22.7	-2.8



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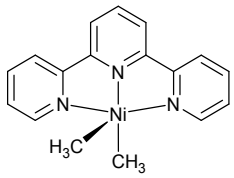
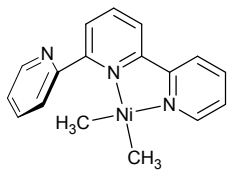


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.525823	0.516685	-5.690459
2	6	0	0.220257	0.165611	-4.710381
3	7	0	-0.564984	-0.714593	-2.186103
4	6	0	1.078782	0.287485	-3.622817
5	6	0	-1.035111	-0.400172	-4.516579
6	6	0	-1.381435	-0.820223	-3.234004
7	6	0	0.647258	-0.167321	-2.377169
8	1	0	2.054066	0.748150	-3.735391
9	1	0	-1.737529	-0.512551	-5.334517
10	1	0	-2.355835	-1.258422	-3.034766
11	6	0	1.495647	-0.074597	-1.160447
12	6	0	2.890036	-0.072659	1.200998
13	6	0	2.890036	-0.072659	-1.200998
14	7	0	0.829048	-0.041311	0.000000

15	6	0	1.495647	-0.074597	1.160447
16	6	0	3.590143	-0.055885	0.000000
17	1	0	3.414404	-0.118518	-2.148548
18	1	0	4.674836	-0.066869	0.000000
19	1	0	3.414404	-0.118518	2.148548
20	6	0	0.647258	-0.167321	2.377169
21	6	0	-1.035111	-0.400172	4.516579
22	6	0	1.078782	0.287485	3.622817
23	7	0	-0.564984	-0.714593	2.186103
24	6	0	-1.381435	-0.820223	3.234004
25	6	0	0.220257	0.165611	4.710381
26	1	0	2.054066	0.748150	3.735391
27	1	0	-2.355835	-1.258422	3.034766
28	1	0	0.525823	0.516685	5.690459
29	1	0	-1.737529	-0.512551	5.334517
30	28	0	-1.222333	0.147427	-0.000000
31	6	0	-3.154895	0.080261	-0.000000
32	1	0	-3.607348	0.543422	0.887300
33	1	0	-3.437994	-0.989463	-0.000000
34	1	0	-3.607348	0.543422	-0.887300
35	6	0	-1.230004	2.116242	-0.000000
36	1	0	-0.206599	2.520603	-0.000000
37	1	0	-1.751155	2.501266	0.885979
38	1	0	-1.751155	2.501266	-0.885979

Zero-point correction= 0.302117
(Hartree/Particle)
Thermal correction to Energy= 0.320693
Thermal correction to Enthalpy= 0.321638
Thermal correction to Gibbs Free Energy= 0.254604
Sum of electronic and zero-point Energies= -990.918473
Sum of electronic and thermal Energies= -990.899896
Sum of electronic and thermal Enthalpies= -990.898952
Sum of electronic and thermal Free Energies= -990.965986

I-bic

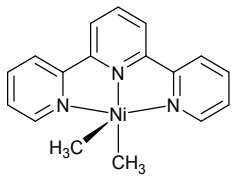


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.661911	0.179809	0.662735
2	6	0	-4.723407	0.037522	0.136831
3	7	0	-2.298852	-0.335340	-1.202160
4	6	0	-3.616045	0.818813	0.446356
5	6	0	-4.600938	-0.932092	-0.852167
6	6	0	-3.370849	-1.072268	-1.492638
7	6	0	-2.423707	0.586371	-0.241046
8	1	0	-3.663260	1.572608	1.225720
9	1	0	-5.436455	-1.565403	-1.128258
10	1	0	-3.241953	-1.812675	-2.278012
11	6	0	-1.209154	1.401919	0.036688
12	6	0	1.085573	2.886925	0.250930
13	6	0	-1.306621	2.785548	0.194061
14	7	0	-0.025548	0.775283	0.045201
15	6	0	1.104208	1.501919	0.089617

16	6	0	-0.142842	3.530286	0.330354
17	1	0	-2.278931	3.264952	0.174379
18	1	0	-0.189310	4.606433	0.458253
19	1	0	2.004093	3.457282	0.306829
20	6	0	2.357949	0.725085	-0.109029
21	6	0	4.545060	-0.848615	-0.610290
22	6	0	3.615268	1.319961	-0.193997
23	7	0	2.192104	-0.603279	-0.254905
24	6	0	3.259166	-1.366761	-0.495276
25	6	0	4.723119	0.519656	-0.449193
26	1	0	3.736398	2.389081	-0.072099
27	1	0	3.068012	-2.430149	-0.588734
28	1	0	5.709969	0.963699	-0.524768
29	1	0	5.378825	-1.509301	-0.816500
30	28	0	0.338283	-1.256031	0.396110
31	6	0	0.865786	-3.127716	0.526562
32	1	0	1.697986	-3.246506	1.238420
33	1	0	1.226713	-3.468039	-0.458925
34	1	0	0.063488	-3.804996	0.837959
35	6	0	-1.220210	-1.627966	1.517709
36	1	0	-1.653778	-0.701405	1.925146
37	1	0	-0.949310	-2.271958	2.364321
38	1	0	-2.010567	-2.142731	0.952668

Zero-point correction= 0.304847
(Hartree/Particle)
Thermal correction to Energy= 0.323834
Thermal correction to Enthalpy= 0.324778
Thermal correction to Gibbs Free Energy= 0.257423
Sum of electronic and zero-point Energies= -990.932977
Sum of electronic and thermal Energies= -990.913990
Sum of electronic and thermal Enthalpies= -990.913045
Sum of electronic and thermal Free Energies= -990.980401

It

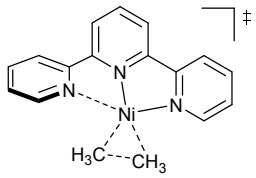


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.759240	0.640742	-0.316175
2	6	0	4.740849	0.268571	-0.278586
3	7	0	2.134831	-0.667579	-0.188849
4	6	0	3.675283	1.160015	-0.209282
5	6	0	4.483199	-1.097578	-0.302783
6	6	0	3.156998	-1.517894	-0.255925
7	6	0	2.376528	0.653438	-0.164508
8	1	0	3.860271	2.227411	-0.196908
9	1	0	5.284873	-1.824711	-0.358823
10	1	0	2.890796	-2.570986	-0.272520
11	6	0	1.167629	1.523278	-0.093473
12	6	0	-1.197993	2.916617	0.031018
13	6	0	1.210021	2.912883	0.031232
14	7	0	0.003004	0.873259	-0.151379
15	6	0	-1.159744	1.526954	-0.093505
16	6	0	0.007096	3.607504	0.093178

17	1	0	2.150457	3.446987	0.087853
18	1	0	0.008786	4.687385	0.194746
19	1	0	-2.136883	3.453518	0.087080
20	6	0	-2.371156	0.660673	-0.164824
21	6	0	-4.480928	-1.086664	-0.305399
22	6	0	-3.669098	1.169597	-0.205349
23	7	0	-2.132210	-0.660595	-0.193596
24	6	0	-3.155387	-1.509470	-0.262259
25	6	0	-4.736132	0.279899	-0.275602
26	1	0	-3.852437	2.237226	-0.188574
27	1	0	-2.889997	-2.562791	-0.282936
28	1	0	-5.754030	0.653764	-0.309603
29	1	0	-5.284049	-1.812107	-0.362542
30	28	0	-0.002890	-1.269551	0.145282
31	6	0	-0.006498	-0.932298	2.203677
32	1	0	-0.888843	-0.344481	2.502605
33	1	0	0.881540	-0.356334	2.508716
34	1	0	-0.014890	-1.857642	2.797229
35	6	0	-0.021347	-3.253812	-0.483157
36	1	0	-0.103202	-3.369402	-1.576265
37	1	0	-0.870191	-3.805230	-0.050352
38	1	0	0.884186	-3.801798	-0.181389

Zero-point correction= 0.301910
(Hartree/Particle)
Thermal correction to Energy= 0.322070
Thermal correction to Enthalpy= 0.323014
Thermal correction to Gibbs Free Energy= 0.251732
Sum of electronic and zero-point Energies= -990.947206
Sum of electronic and thermal Energies= -990.927046
Sum of electronic and thermal Enthalpies= -990.926102
Sum of electronic and thermal Free Energies= -990.997384

TS-1s



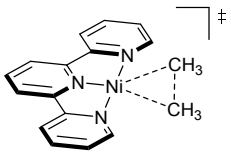
Imaginary frequency = -633.4093 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.669949	0.508379	0.352253
2	6	0	-4.647590	0.224794	0.125688
3	7	0	-2.006554	-0.526290	-0.442633
4	6	0	-3.619408	1.138922	0.252882
5	6	0	-4.341394	-1.083012	-0.284547
6	6	0	-3.023824	-1.405704	-0.543162
7	6	0	-2.305826	0.744411	-0.043412
8	1	0	-3.812503	2.149230	0.598901
9	1	0	-5.116816	-1.830364	-0.408931
10	1	0	-2.746403	-2.407182	-0.863404
11	6	0	-1.142917	1.616405	0.055546
12	6	0	1.256371	2.968439	-0.045613
13	6	0	-1.152286	3.001820	-0.068364
14	7	0	0.021726	0.926766	0.215374

15	6	0	1.206681	1.584461	0.078480
16	6	0	0.061702	3.690504	-0.090544
17	1	0	-2.091243	3.533605	-0.184804
18	1	0	0.077880	4.768306	-0.207465
19	1	0	2.210987	3.475079	-0.145045
20	6	0	2.348650	0.682666	-0.005165
21	6	0	4.354597	-1.173956	-0.267659
22	6	0	3.670732	1.056559	0.278710
23	7	0	2.024196	-0.587287	-0.388087
24	6	0	3.029013	-1.477865	-0.508266
25	6	0	4.683881	0.126967	0.143911
26	1	0	3.882940	2.065691	0.616530
27	1	0	2.737096	-2.473264	-0.831566
28	1	0	5.712484	0.395756	0.360022
29	1	0	5.117329	-1.931992	-0.404460
30	28	0	0.002914	-1.021299	-0.045943
31	6	0	-0.036067	-3.002070	-0.265990
32	1	0	0.911956	-3.521568	-0.128950
33	1	0	-0.114462	-2.684937	-1.326753
34	1	0	-0.855571	-3.697175	-0.079630
35	6	0	-0.275598	-2.277125	1.590095
36	1	0	0.226842	-1.475898	2.143437
37	1	0	0.124601	-3.229134	1.932403
38	1	0	-1.352653	-2.237787	1.755735

Zero-point correction= 0.303566
(Hartree/Particle)
Thermal correction to Energy= 0.322111
Thermal correction to Enthalpy= 0.323055
Thermal correction to Gibbs Free Energy= 0.257013
Sum of electronic and zero-point Energies= -990.869130
Sum of electronic and thermal Energies= -990.850585
Sum of electronic and thermal Enthalpies= -990.849641
Sum of electronic and thermal Free Energies= -990.915683

TS-1t



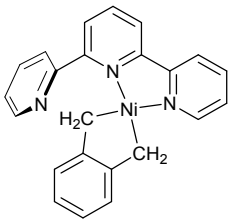
Imaginary frequency = -229.9249 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.765823	0.712030	-0.012132
2	6	0	-4.744286	0.344817	-0.012241
3	7	0	-2.122954	-0.602570	-0.016517
4	6	0	-3.692217	1.231477	-0.014341
5	6	0	-4.484007	-1.041706	-0.008548
6	6	0	-3.163362	-1.446585	-0.011160
7	6	0	-2.362908	0.745088	-0.013540
8	1	0	-3.881247	2.299340	-0.015156
9	1	0	-5.285187	-1.771087	-0.004054
10	1	0	-2.904191	-2.503916	-0.007237
11	6	0	-1.188209	1.582185	-0.005489
12	6	0	1.219324	2.967564	0.017178
13	6	0	-1.195555	2.989089	0.001738

14	7	0	0.006453	0.903526	-0.002272
15	6	0	1.175809	1.589502	0.007960
16	6	0	-0.002664	3.682256	0.013675
17	1	0	-2.135034	3.531484	-0.000869
18	1	0	0.002411	4.766568	0.020691
19	1	0	2.160401	3.503888	0.027837
20	6	0	2.383125	0.727431	0.005201
21	6	0	4.496401	-1.038098	-0.015931
22	6	0	3.691306	1.224152	-0.005007
23	7	0	2.142895	-0.599256	0.007006
24	6	0	3.171835	-1.450593	-0.005033
25	6	0	4.754276	0.333406	-0.014732
26	1	0	3.876130	2.291707	-0.007832
27	1	0	2.911013	-2.506268	-0.007579
28	1	0	5.774356	0.703283	-0.023173
29	1	0	5.298386	-1.766936	-0.025899
30	28	0	-0.020422	-1.121799	0.000294
31	6	0	0.031562	-2.753276	-1.130825
32	1	0	0.778844	-3.530425	-0.979320
33	1	0	0.300677	-2.140982	-2.004350
34	1	0	-0.959267	-3.187070	-1.262982
35	6	0	-0.034669	-2.716474	1.183764
36	1	0	-0.291166	-2.080154	2.043233
37	1	0	0.957360	-3.148552	1.314020
38	1	0	-0.785191	-3.495828	1.063061

Zero-point correction= 0.301963
(Hartree/Particle)
Thermal correction to Energy= 0.320896
Thermal correction to Enthalpy= 0.321840
Thermal correction to Gibbs Free Energy= 0.253646
Sum of electronic and zero-point Energies= -990.921736
Sum of electronic and thermal Energies= -990.902803
Sum of electronic and thermal Enthalpies= -990.901859
Sum of electronic and thermal Free Energies= -990.970053

IIs

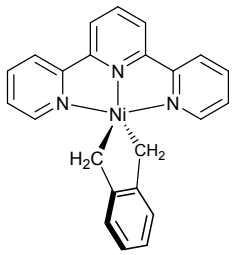


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.083244	-0.662029	0.249843
2	7	0	-1.316256	0.987704	-0.176004
3	6	0	-2.910578	2.621030	-1.757679
4	6	0	-0.944879	2.248733	-0.433688
5	6	0	-2.516820	0.560086	-0.607730
6	6	0	-3.337937	1.344261	-1.415873
7	6	0	-1.711932	3.092588	-1.239516
8	1	0	-4.285755	0.968170	-1.779967
9	1	0	-1.380799	4.108301	-1.424941
10	1	0	-3.523278	3.251756	-2.392641
11	7	0	0.381886	2.460673	1.547130
12	6	0	2.325947	3.994824	0.251213
13	6	0	1.452668	2.914530	2.197604

14	6	0	0.274465	2.762097	0.248274
15	6	0	1.209350	3.536436	-0.439020
16	6	0	2.455424	3.675542	1.598122
17	1	0	1.514905	2.657636	3.252175
18	1	0	1.077128	3.745133	-1.495699
19	1	0	3.309506	4.006513	2.178214
20	1	0	3.084198	4.582222	-0.256316
21	7	0	-1.941581	-1.471325	0.509612
22	6	0	-4.503203	-2.518517	0.352212
23	6	0	-2.915839	-0.784412	-0.113239
24	6	0	-2.225698	-2.653282	1.058945
25	6	0	-3.497084	-3.214638	1.011502
26	6	0	-4.212501	-1.283914	-0.217639
27	1	0	-1.399975	-3.162002	1.544336
28	1	0	-3.683088	-4.174229	1.478881
29	1	0	-4.990021	-0.718218	-0.716116
30	1	0	-5.506994	-2.924631	0.287287
31	6	0	0.856311	-2.359776	0.510634
32	1	0	0.293622	-3.188037	0.050274
33	1	0	0.881525	-2.576992	1.593692
34	6	0	1.663420	0.070926	-0.287414
35	1	0	1.570439	0.683254	-1.200779
36	1	0	2.037692	0.758050	0.487528
37	6	0	2.665010	-1.038618	-0.489711
38	6	0	4.379658	-3.241966	-0.749877
39	6	0	2.252881	-2.303289	-0.052652
40	6	0	3.936222	-0.889278	-1.056597
41	6	0	4.790238	-1.983001	-1.190780
42	6	0	3.115698	-3.396675	-0.181680
43	1	0	4.256045	0.093009	-1.401307
44	1	0	5.771965	-1.856967	-1.639873
45	1	0	2.789750	-4.379326	0.156030
46	1	0	5.040710	-4.098335	-0.853998

Zero-point correction=	0.367060
(Hartree/Particle)	
Thermal correction to Energy=	0.388985
Thermal correction to Enthalpy=	0.389929
Thermal correction to Gibbs Free Energy=	0.315346
Sum of electronic and zero-point Energies=	-1220.641926
Sum of electronic and thermal Energies=	-1220.620001
Sum of electronic and thermal Enthalpies=	-1220.619057
Sum of electronic and thermal Free Energies=	-1220.693640

IIt

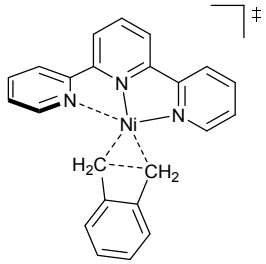


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.128304	-0.594364	-0.377619
2	7	0	1.308965	1.161272	-0.068425
3	6	0	2.810561	3.397735	0.467049

4	6	0	0.711274	2.354791	-0.017930
5	6	0	2.624433	1.036755	0.134733
6	6	0	3.418776	2.148750	0.412367
7	6	0	1.443371	3.513376	0.248696
8	1	0	4.484931	2.053970	0.576177
9	1	0	0.968249	4.485693	0.283020
10	1	0	3.403217	4.281461	0.677427
11	7	0	-1.287378	1.143881	-0.573582
12	6	0	-2.917181	3.382350	-0.346832
13	6	0	-2.604088	1.050087	-0.770161
14	6	0	-0.759912	2.339125	-0.255386
15	6	0	-1.546001	3.483626	-0.134928
16	6	0	-3.458873	2.145166	-0.667826
17	1	0	-2.983977	0.059660	-1.003191
18	1	0	-1.106988	4.437873	0.129191
19	1	0	-4.522196	2.015101	-0.832875
20	1	0	-3.548537	4.260133	-0.256178
21	7	0	2.246973	-1.288137	-0.305554
22	6	0	4.888109	-2.002683	0.134926
23	6	0	3.150955	-0.353704	0.031890
24	6	0	2.635715	-2.556124	-0.430265
25	6	0	3.949816	-2.963868	-0.221032
26	6	0	4.486999	-0.677317	0.263947
27	1	0	1.859346	-3.262725	-0.707585
28	1	0	4.220994	-4.006926	-0.333858
29	1	0	5.205690	0.082974	0.544892
30	1	0	5.922776	-2.276780	0.311929
31	6	0	-0.901243	-2.315786	-1.051646
32	1	0	-0.264076	-3.110471	-0.631577
33	1	0	-1.131657	-2.586033	-2.089607
34	6	0	-0.601840	-1.255576	1.493428
35	1	0	0.010671	-2.160101	1.622692
36	1	0	-0.573874	-0.666143	2.417234
37	6	0	-1.984018	-1.568312	1.057868
38	6	0	-4.566366	-1.976053	-0.013765
39	6	0	-2.138031	-2.147432	-0.241172
40	6	0	-3.132547	-1.189543	1.759576
41	6	0	-4.415534	-1.375150	1.232051
42	6	0	-3.429360	-2.364694	-0.732387
43	1	0	-3.017448	-0.717179	2.734274
44	1	0	-5.287315	-1.057760	1.798587
45	1	0	-3.545543	-2.806767	-1.721113
46	1	0	-5.556765	-2.136000	-0.432385

Zero-point correction= 0.365781
(Hartree/Particle)
Thermal correction to Energy= 0.387800
Thermal correction to Enthalpy= 0.388745
Thermal correction to Gibbs Free Energy= 0.313034
Sum of electronic and zero-point Energies= -1220.657297
Sum of electronic and thermal Energies= -1220.635277
Sum of electronic and thermal Enthalpies= -1220.634333
Sum of electronic and thermal Free Energies= -1220.710044

TS-(II-IV)s



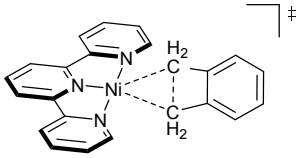
Imaginary frequency = -513.7289 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.162514	-0.191912	-0.234089
2	7	0	-1.754208	0.710996	0.307407
3	6	0	-4.188411	2.083235	0.195492
4	6	0	-2.942029	0.021296	0.190491
5	6	0	-1.780567	2.083534	0.179789
6	6	0	-2.976550	2.783734	0.164176
7	6	0	-4.161405	0.687466	0.171976
8	1	0	-2.968731	3.866501	0.085187
9	1	0	-5.085234	0.121922	0.097909
10	1	0	-5.131649	2.615850	0.158917
11	7	0	-1.485613	-1.746505	-0.388675
12	6	0	-3.430176	-3.705132	0.157415
13	6	0	-1.215616	-3.067092	-0.501650
14	6	0	-2.746150	-1.397493	0.034518
15	6	0	-3.724982	-2.370538	0.315739
16	6	0	-2.133190	-4.064724	-0.260711
17	1	0	-0.208561	-3.320753	-0.818320
18	1	0	-4.697493	-2.054037	0.678161
19	1	0	-1.852636	-5.101907	-0.402692
20	1	0	-4.174645	-4.465607	0.368118
21	7	0	0.468891	1.741230	-0.433463
22	6	0	1.181991	4.404104	0.071416
23	6	0	-0.462106	2.647725	0.003971
24	6	0	1.739781	2.169891	-0.593765
25	6	0	2.137307	3.471370	-0.373215
26	6	0	-0.115956	3.984256	0.269315
27	1	0	2.455223	1.423262	-0.929017
28	1	0	3.167883	3.758099	-0.547556
29	1	0	-0.870680	4.666261	0.646767
30	1	0	1.464879	5.432242	0.271542
31	6	0	1.569773	-1.102949	-1.014192
32	1	0	1.363525	-0.355474	-1.792470
33	1	0	1.234721	-2.078796	-1.371951
34	6	0	1.373418	-1.151813	1.003553
35	1	0	0.990607	-0.391001	1.689860
36	1	0	0.926455	-2.123870	1.226299
37	6	0	2.862055	-1.163991	0.828828
38	6	0	5.361508	-1.151157	-0.321563
39	6	0	2.998516	-1.120701	-0.544824
40	6	0	3.961706	-1.210047	1.673710
41	6	0	5.223656	-1.199861	1.068499
42	6	0	4.241962	-1.113065	-1.160779
43	1	0	3.860777	-1.240240	2.754734
44	1	0	6.114565	-1.222022	1.688682

45	1	0	4.353798	-1.068585	-2.240495
46	1	0	6.356902	-1.136655	-0.755207

Zero-point correction= 0.364451
(Hartree/Particle)
Thermal correction to Energy= 0.385925
Thermal correction to Enthalpy= 0.386869
Thermal correction to Gibbs Free Energy= 0.313422
Sum of electronic and zero-point Energies= -1220.559307
Sum of electronic and thermal Energies= -1220.537834
Sum of electronic and thermal Enthalpies= -1220.536890
Sum of electronic and thermal Free Energies= -1220.610337

TS-(II-IV)t



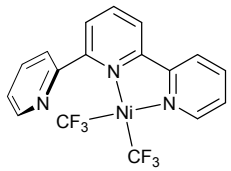
Imaginary frequency = -333.2421 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.065041	-0.318773	-0.000124
2	7	0	1.743789	0.810526	0.000013
3	6	0	4.073590	2.306462	0.000260
4	6	0	1.680070	2.156295	0.000113
5	6	0	2.955939	0.165154	0.000032
6	6	0	4.146122	0.934082	0.000160
7	6	0	2.808222	2.950550	0.000238
8	1	0	5.114473	0.444701	0.000176
9	1	0	2.747016	4.031585	0.000317
10	1	0	4.981004	2.901096	0.000354
11	7	0	-0.692367	1.776851	-0.000040
12	6	0	-1.325779	4.475916	0.000086
13	6	0	-1.966478	2.178987	-0.000089
14	6	0	0.291224	2.697446	0.000073
15	6	0	0.000220	4.064379	0.000139
16	6	0	-2.336676	3.517557	-0.000030
17	1	0	-2.713101	1.387091	-0.000184
18	1	0	0.797968	4.797373	0.000231
19	1	0	-3.384050	3.795925	-0.000075
20	1	0	-1.567403	5.533831	0.000134
21	7	0	1.620619	-1.813286	-0.000213
22	6	0	3.865581	-3.480417	-0.000215
23	6	0	2.886158	-1.267115	-0.000090
24	6	0	1.498798	-3.148008	-0.000334
25	6	0	2.562105	-4.029222	-0.000345
26	6	0	4.023920	-2.116720	-0.000090
27	1	0	0.475451	-3.522044	-0.000425
28	1	0	2.392793	-5.099182	-0.000445
29	1	0	5.019657	-1.686549	0.000015
30	1	0	4.735754	-4.129635	-0.000214
31	6	0	-1.454840	-1.250566	-1.054870
32	1	0	-1.048491	-2.224402	-1.343477
33	1	0	-1.183954	-0.498180	-1.810357
34	6	0	-1.454657	-1.250717	1.054740
35	1	0	-1.048262	-2.224604	1.343110
36	1	0	-1.183631	-0.498461	1.810306

37	6	0	-2.911712	-1.286047	0.691522
38	6	0	-5.289578	-1.353082	-0.698415
39	6	0	-2.911833	-1.285962	-0.691402
40	6	0	-4.091667	-1.323602	1.421789
41	6	0	-5.289453	-1.353166	0.698959
42	6	0	-4.091922	-1.323428	-1.421459
43	1	0	-4.096016	-1.317286	2.508172
44	1	0	-6.236032	-1.370035	1.230656
45	1	0	-4.096470	-1.316979	-2.507841
46	1	0	-6.236253	-1.369886	-1.229945

Zero-point correction= 0.363330
(Hartree/Particle)
Thermal correction to Energy= 0.385402
Thermal correction to Enthalpy= 0.386346
Thermal correction to Gibbs Free Energy= 0.309166
Sum of electronic and zero-point Energies= -1220.616947
Sum of electronic and thermal Energies= -1220.594874
Sum of electronic and thermal Enthalpies= -1220.593930
Sum of electronic and thermal Free Energies= -1220.671111

IIIs

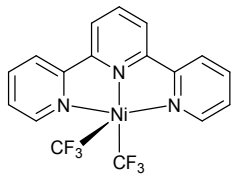


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.377269	-0.603828	0.038948
2	9	0	-1.517441	-0.008175	1.958091
3	9	0	-2.194532	-1.668865	0.752882
4	9	0	1.841081	-2.881808	0.672022
5	9	0	1.266115	-2.696145	-1.409180
6	9	0	-0.159277	-3.400944	0.044666
7	9	0	-0.629290	-1.951007	2.214619
8	7	0	0.021511	1.381207	-0.024198
9	7	0	-2.067318	0.228028	-1.438557
10	7	0	2.246265	0.080447	-0.456962
11	6	0	1.133432	2.118611	0.125530
12	6	0	-3.596957	1.309706	0.069554
13	6	0	-1.315085	3.341832	0.162399
14	6	0	-4.636570	0.506574	-0.383900
15	6	0	-2.331121	1.131473	-0.487125
16	6	0	2.400150	1.367884	-0.078875
17	6	0	-0.176843	4.097054	0.413068
18	6	0	0.808610	-2.467651	-0.124623
19	6	0	-3.073641	-0.535259	-1.862829
20	6	0	1.072447	3.489000	0.365832
21	6	0	3.331071	-0.645751	-0.742059
22	6	0	-4.373619	-0.434431	-1.373103
23	6	0	3.657824	1.949582	0.043825
24	6	0	4.619618	-0.127776	-0.662667
25	6	0	4.783683	1.187951	-0.251153
26	6	0	-1.064927	-1.093150	1.240502
27	6	0	-1.177824	1.973756	-0.071938
28	1	0	-3.753169	2.038757	0.857547
29	1	0	-2.293451	3.805285	0.108896

30	1	0	-5.632364	0.609954	0.034573
31	1	0	-0.256332	5.162718	0.598879
32	1	0	-2.829800	-1.262235	-2.633245
33	1	0	1.972235	4.077123	0.494825
34	1	0	3.151986	-1.670107	-1.041149
35	1	0	-5.152697	-1.083284	-1.756991
36	1	0	3.764506	2.978078	0.365264
37	1	0	5.467703	-0.753580	-0.912767
38	1	0	5.773253	1.622775	-0.160915

Zero-point correction= 0.261520
(Hartree/Particle)
Thermal correction to Energy= 0.284475
Thermal correction to Enthalpy= 0.285419
Thermal correction to Gibbs Free Energy= 0.208821
Sum of electronic and zero-point Energies= -1586.299087
Sum of electronic and thermal Energies= -1586.276131
Sum of electronic and thermal Enthalpies= -1586.275187
Sum of electronic and thermal Free Energies= -1586.351786

IIIt

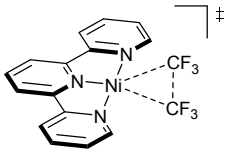


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.050808	-0.606141	-0.260836
2	9	0	-0.981586	0.409727	2.243589
3	9	0	-1.084602	-1.749079	2.153919
4	9	0	1.050387	-3.243167	0.270865
5	9	0	0.949373	-2.889025	-1.856367
6	9	0	-0.843102	-3.417237	-0.760195
7	9	0	0.791689	-0.775403	2.615375
8	7	0	-0.012166	1.471934	-0.351570
9	7	0	-2.051644	-0.158457	-0.551454
10	7	0	2.134301	-0.026177	-0.297616
11	6	0	1.131427	2.151545	-0.257713
12	6	0	-3.687492	1.572140	-0.379485
13	6	0	-1.290002	3.461336	-0.231488
14	6	0	-4.701902	0.621814	-0.459447
15	6	0	-2.364265	1.144169	-0.426309
16	6	0	2.356873	1.300593	-0.266315
17	6	0	-0.108292	4.190460	-0.138844
18	6	0	0.273324	-2.614097	-0.681924
19	6	0	-3.021575	-1.068792	-0.619431
20	6	0	1.122841	3.541478	-0.147978
21	6	0	3.164217	-0.871077	-0.299660
22	6	0	-4.369315	-0.721629	-0.580636
23	6	0	3.647710	1.820267	-0.242261
24	6	0	4.484551	-0.430876	-0.273909
25	6	0	4.724538	0.937556	-0.246573
26	6	0	-0.290102	-0.693715	1.775559
27	6	0	-1.201615	2.073358	-0.334319
28	1	0	-3.930080	2.622881	-0.276128
29	1	0	-2.246421	3.969451	-0.220252
30	1	0	-5.740480	0.933252	-0.424450

31	1	0	-0.147327	5.271114	-0.054835
32	1	0	-2.690851	-2.099351	-0.704232
33	1	0	2.041802	4.108412	-0.064520
34	1	0	2.908876	-1.925903	-0.317113
35	1	0	-5.130669	-1.490101	-0.642615
36	1	0	3.818284	2.889960	-0.223440
37	1	0	5.296384	-1.148479	-0.275876
38	1	0	5.739465	1.320077	-0.228922

Zero-point correction= 0.259634
(Hartree/Particle)
Thermal correction to Energy= 0.283484
Thermal correction to Enthalpy= 0.284429
Thermal correction to Gibbs Free Energy= 0.203226
Sum of electronic and zero-point Energies= -1586.312544
Sum of electronic and thermal Energies= -1586.288693
Sum of electronic and thermal Enthalpies= -1586.287749
Sum of electronic and thermal Free Energies= -1586.368952

TS-(III-IV)t



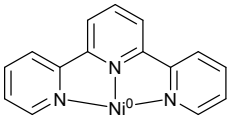
Imaginary frequency = -271.2748 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.018968	-0.312613	-0.021160
2	9	0	-0.772968	-1.565817	1.921942
3	9	0	-0.513728	-3.479885	1.051628
4	9	0	1.032022	-3.289223	-0.843725
5	9	0	0.555361	-1.543745	-1.956203
6	9	0	-1.044367	-2.805756	-1.268385
7	9	0	1.227565	-2.281788	1.501725
8	7	0	-0.039049	1.674820	-0.001521
9	7	0	-2.103997	0.063062	-0.099971
10	7	0	2.103381	0.170304	-0.014873
11	6	0	1.110870	2.367886	0.050881
12	6	0	-3.732000	1.860619	-0.087321
13	6	0	-1.294091	3.713985	0.043823
14	6	0	-4.760180	0.951521	-0.110728
15	6	0	-2.385019	1.416052	-0.071514
16	6	0	2.323881	1.503862	0.020416
17	6	0	-0.116960	4.423482	0.107469
18	6	0	0.133936	-2.305742	-0.926609
19	6	0	-3.132919	-0.800654	-0.111386
20	6	0	1.131260	3.746119	0.109738
21	6	0	3.153060	-0.655955	-0.085856
22	6	0	-4.461407	-0.430627	-0.116521
23	6	0	3.620044	2.022921	0.005417
24	6	0	4.468530	-0.215173	-0.111360
25	6	0	4.702451	1.156613	-0.058271
26	6	0	-0.019146	-2.244299	1.047643
27	6	0	-1.256391	2.299599	-0.012058
28	1	0	-3.945688	2.924019	-0.076590
29	1	0	-2.242222	4.241148	0.040531
30	1	0	-5.790691	1.292638	-0.121020

31	1	0	-0.138665	5.507098	0.155143
32	1	0	-2.859574	-1.852853	-0.116352
33	1	0	2.056180	4.307048	0.157550
34	1	0	2.924951	-1.716627	-0.122222
35	1	0	-5.240808	-1.182936	-0.127225
36	1	0	3.779646	3.093889	0.035583
37	1	0	5.280575	-0.930085	-0.171203
38	1	0	5.714579	1.547190	-0.072576

Zero-point correction= 0.258689
(Hartree/Particle)
Thermal correction to Energy= 0.281127
Thermal correction to Enthalpy= 0.282071
Thermal correction to Gibbs Free Energy= 0.205105
Sum of electronic and zero-point Energies= -1586.221922
Sum of electronic and thermal Energies= -1586.199484
Sum of electronic and thermal Enthalpies= -1586.198540
Sum of electronic and thermal Free Energies= -1586.275506

IVs

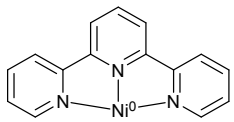


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.050701	0.171441	5.684847
2	6	0	0.218900	0.097176	4.636419
3	7	0	0.925805	-0.123780	1.944699
4	6	0	-0.752129	0.159261	3.661795
5	6	0	1.568290	-0.040223	4.255421
6	6	0	1.864732	-0.143476	2.913941
7	6	0	-0.386958	0.062295	2.305544
8	1	0	-1.794615	0.309710	3.921965
9	1	0	2.361912	-0.084155	4.991731
10	1	0	2.886713	-0.277228	2.571281
11	6	0	-1.294969	0.149543	1.187791
12	6	0	-2.644646	-0.164840	-1.203870
13	6	0	-2.644646	-0.164840	1.203870
14	7	0	-0.651045	0.486837	0.000000
15	6	0	-1.294969	0.149543	-1.187791
16	6	0	-3.353023	-0.262717	0.000000
17	1	0	-3.134761	-0.387778	2.147112
18	1	0	-4.404069	-0.526262	0.000000
19	1	0	-3.134761	-0.387778	-2.147112
20	6	0	-0.386958	0.062295	-2.305544
21	6	0	1.568290	-0.040223	-4.255421
22	6	0	-0.752129	0.159261	-3.661795
23	7	0	0.925805	-0.123780	-1.944699
24	6	0	1.864732	-0.143476	-2.913941
25	6	0	0.218900	0.097176	-4.636419
26	1	0	-1.794615	0.309710	-3.921965
27	1	0	2.886713	-0.277228	-2.571281
28	1	0	-0.050701	0.171441	-5.684847
29	1	0	2.361912	-0.084155	-4.991731
30	28	0	1.167947	-0.016900	-0.000000

Zero-point correction= 0.229212
(Hartree/Particle)

Thermal correction to Energy= 0.243359
Thermal correction to Enthalpy= 0.244303
Thermal correction to Gibbs Free Energy= 0.188082
Sum of electronic and zero-point Energies= -911.235903
Sum of electronic and thermal Energies= -911.221756
Sum of electronic and thermal Enthalpies= -911.220812
Sum of electronic and thermal Free Energies= -911.277032

IVt



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.264800	0.000024	5.741122
2	6	0	-0.078129	0.000018	4.711564
3	7	0	-0.959125	-0.000005	2.058393
4	6	0	0.832393	-0.000011	3.674469
5	6	0	-1.450685	0.000038	4.414019
6	6	0	-1.826742	0.000023	3.083910
7	6	0	0.382608	-0.000016	2.342249
8	1	0	1.896852	-0.000031	3.881748
9	1	0	-2.202435	0.000063	5.194487
10	1	0	-2.877602	0.000030	2.807371
11	6	0	1.282080	-0.000034	1.188017
12	6	0	2.671693	0.000022	-1.215805
13	6	0	2.671693	0.000022	1.215805
14	7	0	0.626537	-0.000091	-0.000000
15	6	0	1.282080	-0.000034	-1.188017
16	6	0	3.370380	0.000037	-0.000000
17	1	0	3.218712	0.000068	2.152942
18	1	0	4.454609	0.000082	-0.000000
19	1	0	3.218712	0.000068	-2.152942
20	6	0	0.382608	-0.000016	-2.342249
21	6	0	-1.450685	0.000038	-4.414019
22	6	0	0.832393	-0.000011	-3.674469
23	7	0	-0.959125	-0.000005	-2.058393
24	6	0	-1.826742	0.000023	-3.083910
25	6	0	-0.078129	0.000018	-4.711564
26	1	0	1.896852	-0.000031	-3.881748
27	1	0	-2.877602	0.000030	-2.807371
28	1	0	0.264800	0.000024	-5.741122
29	1	0	-2.202435	0.000063	-5.194487
30	28	0	-1.356935	-0.000014	0.000000

Zero-point correction= 0.226755
(Hartree/Particle)
ethene Thermal correction to Energy= 0.241239
Thermal correction to Enthalpy= 0.242183
Thermal correction to Gibbs Free Energy= 0.183810
Sum of electronic and zero-point Energies= -911.291916
Sum of electronic and thermal Energies= -911.277432
Sum of electronic and thermal Enthalpies= -911.276488
Sum of electronic and thermal Free Energies= -911.334861

Ethane

$H_3C—CH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.019507	1.159380
2	6	0	0.000000	0.000000	0.763044
3	1	0	0.882919	-0.509754	1.159380
4	1	0	-0.882919	-0.509753	1.159380
5	6	0	-0.000000	-0.000000	-0.763044
6	1	0	0.882919	0.509753	-1.159380
7	1	0	-0.882919	0.509754	-1.159380
8	1	0	-0.000000	-1.019507	-1.159380

Zero-point correction= 0.075553
(Hartree/Particle)
Thermal correction to Energy= 0.079053
Thermal correction to Enthalpy= 0.079997
Thermal correction to Gibbs Free Energy= 0.054111
Sum of electronic and zero-point Energies= -79.695553
Sum of electronic and thermal Energies= -79.692053
Sum of electronic and thermal Enthalpies= -79.691109
Sum of electronic and thermal Free Energies= -79.716996

Benzocyclobutane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.523299	-0.733576
2	6	0	0.000000	1.437364	-0.717871
3	6	0	-0.000000	-1.437364	-0.717871
4	6	0	0.000000	0.695817	0.452990
5	6	0	0.000000	0.699930	-1.909293
6	6	0	-0.000000	-0.699930	-1.909293
7	6	0	-0.000000	-0.695817	0.452990
8	1	0	0.000000	1.224243	-2.860551
9	1	0	-0.000000	-1.224243	-2.860551
10	1	0	-0.000000	-2.523299	-0.733576
11	6	0	0.000000	0.785986	1.968854
12	1	0	-0.889880	1.240635	2.413027
13	1	0	0.889880	1.240635	2.413027
14	6	0	-0.000000	-0.785986	1.968854
15	1	0	-0.889880	-1.240635	2.413027
16	1	0	0.889880	-1.240635	2.413027

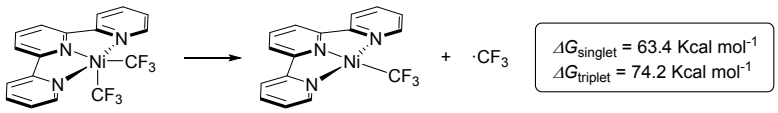
Zero-point correction= 0.136052
(Hartree/Particle)
Thermal correction to Energy= 0.142040
Thermal correction to Enthalpy= 0.142984
Thermal correction to Gibbs Free Energy= 0.106818
Sum of electronic and zero-point Energies= -309.348713
Sum of electronic and thermal Energies= -309.342725
Sum of electronic and thermal Enthalpies= -309.341781
Sum of electronic and thermal Free Energies= -309.377946

Hexafluoroethane

$CF_3—CF_3$

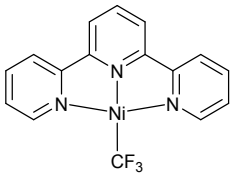
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.765543
2	6	0	-0.000000	-0.000000	-0.765543
3	9	0	1.083323	0.625457	-1.212162
4	9	0	-1.083323	0.625457	-1.212162
5	9	0	0.000000	1.250914	1.212162
6	9	0	1.083323	-0.625457	1.212162
7	9	0	-0.000000	-1.250914	-1.212162
8	9	0	-1.083323	-0.625457	1.212162

Zero-point correction= 0.030472
(Hartree/Particle)
Thermal correction to Energy= 0.037199
Thermal correction to Enthalpy= 0.038143
Thermal correction to Gibbs Free Energy= 0.000270
Sum of electronic and zero-point Energies= -675.008380
Sum of electronic and thermal Energies= -675.001653
Sum of electronic and thermal Enthalpies= -675.000708
Sum of electronic and thermal Free Energies= -675.038582



IIIs or **IIIt**

TPY-Ni-CF_3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.776056	0.494856	0.000653
2	6	0	-4.718669	0.251115	0.000255
3	7	0	-1.988121	-0.402343	-0.000648
4	6	0	-3.776367	1.248337	0.000679
5	6	0	-4.290874	-1.095268	-0.000695
6	6	0	-2.938735	-1.359833	-0.001036
7	6	0	-2.400945	0.923150	0.000111
8	1	0	-4.072753	2.291929	0.001460
9	1	0	-4.998196	-1.915432	-0.001191
10	1	0	-2.573197	-2.376570	-0.001741
11	6	0	-1.343958	1.877638	0.000164
12	6	0	1.003737	3.394002	0.000028
13	6	0	-1.424540	3.286642	-0.000012
14	7	0	-0.107234	1.292453	0.000323

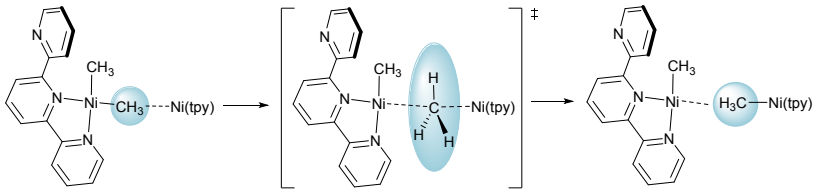
15	6	0	1.030164	2.018680	0.000135
16	6	0	-0.266227	4.032258	-0.000041
17	1	0	-2.391455	3.778727	-0.000215
18	1	0	-0.319508	5.115275	-0.000216
19	1	0	1.914236	3.980499	-0.000034
20	6	0	2.225686	1.156304	0.000042
21	6	0	4.313569	-0.621341	-0.000486
22	6	0	3.531020	1.640785	0.000400
23	7	0	1.960359	-0.178580	-0.000472
24	6	0	2.990171	-1.037731	-0.000761
25	6	0	4.589074	0.743125	0.000139
26	1	0	3.710017	2.709449	0.000879
27	1	0	2.738450	-2.088349	-0.001253
28	1	0	5.612318	1.103080	0.000401
29	1	0	5.105995	-1.360084	-0.000776
30	28	0	-0.015654	-0.597329	-0.000239
31	6	0	0.221177	-2.537102	0.000458
32	9	0	0.969830	-2.936982	1.083176
33	9	0	-0.830999	-3.404252	0.001480
34	9	0	0.968692	-2.938039	-1.082652

Zero-point correction= (Hartree/Particle)	0.245900
Thermal correction to Energy=	0.263335
Thermal correction to Enthalpy=	0.264279
Thermal correction to Gibbs Free Energy=	0.200478
Sum of electronic and zero-point Energies=	-1248.797131
Sum of electronic and thermal Energies=	-1248.779696
Sum of electronic and thermal Enthalpies=	-1248.778752
Sum of electronic and thermal Free Energies=	-1248.842553

·CF_3

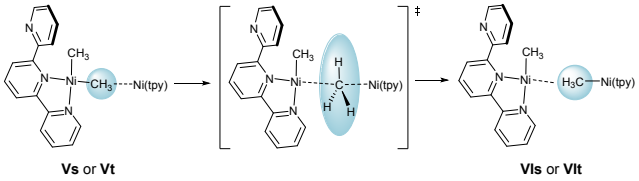
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	9	0	0.000000	1.311603	0.000000
3	9	0	1.135882	-0.655802	0.000000
4	9	0	-1.135882	-0.655802	0.000000

Zero-point correction= (Hartree/Particle)	0.011096
Thermal correction to Energy=	0.014473
Thermal correction to Enthalpy=	0.015417
Thermal correction to Gibbs Free Energy=	-0.013999
Sum of electronic and zero-point Energies=	-337.383031
Sum of electronic and thermal Energies=	-337.379653
Sum of electronic and thermal Enthalpies=	-337.378709
Sum of electronic and thermal Free Energies=	-337.408125

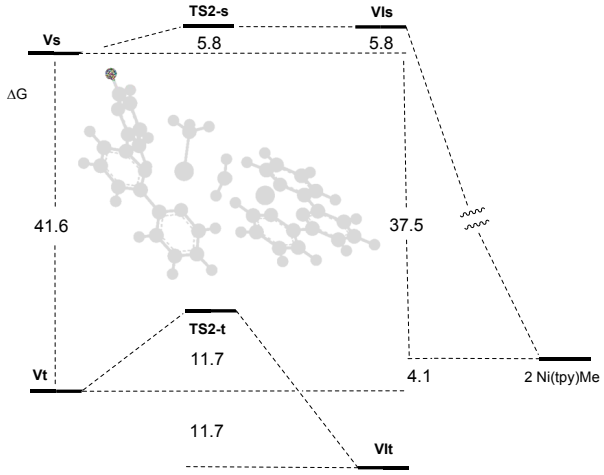


Vs or **Vt** **VIs** or **VIt**

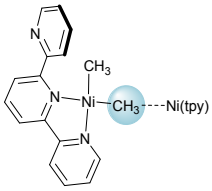
	Vs	**Vt**
ΔG_a	5.84	11.7
ΔG	5.80	-11.7



Vs or **Vt** **VIs** or **VIt**



Vs



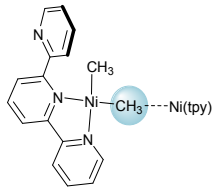
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.201680	-1.417778	-1.584195
2	6	0	6.588289	-1.325798	-1.626885
3	6	0	7.213762	-0.378716	-0.825898
4	7	0	4.451956	-0.642740	-0.797366
5	6	0	6.437412	0.431708	-0.004862
6	6	0	5.053464	0.271490	-0.012518
7	6	0	4.146702	1.040360	0.880870
8	7	0	2.885585	0.571527	0.949288
9	6	0	4.570093	2.136306	1.627093
10	6	0	3.662955	2.742348	2.490458
11	6	0	2.040723	1.095846	1.849463

12	6	0	2.392770	2.203780	2.625351
13	6	0	0.732753	0.425411	2.084455
14	6	0	0.626732	-0.964969	2.019242
15	7	0	-0.286235	1.224354	2.426988
16	6	0	-0.601730	-1.550745	2.312939
17	6	0	-1.460756	0.649153	2.684446
18	6	0	-1.669383	-0.729048	2.649227
19	28	0	2.424782	-0.429270	-0.848628
20	6	0	2.218652	-1.488003	-2.464950
21	6	0	0.544369	0.205026	-1.006901
22	1	0	4.664903	-2.128254	-2.202312
23	1	0	7.154713	-1.982886	-2.275871
24	1	0	8.293318	-0.273287	-0.830931
25	1	0	6.907297	1.161779	0.642379
26	1	0	5.577349	2.521942	1.531380
27	1	0	3.958435	3.608546	3.072706
28	1	0	1.668615	2.607155	3.322254
29	1	0	1.488752	-1.563256	1.740854
30	1	0	-0.729311	-2.628214	2.251577
31	1	0	-2.279902	1.321011	2.928575
32	1	0	-2.654703	-1.138282	2.845681
33	1	0	1.197753	-1.557715	-2.853740
34	1	0	2.565939	-2.511021	-2.247086
35	1	0	2.856221	-1.080291	-3.263058
36	1	0	0.400761	1.129630	-0.439133
37	1	0	0.272615	0.304907	-2.060724
38	1	0	0.094667	-0.661438	-0.506654
39	6	0	-0.964490	-2.924772	-0.666202
40	6	0	-1.091496	-4.216018	-0.219225
41	6	0	-2.291612	-4.588278	0.448585
42	7	0	-1.930820	-1.980542	-0.539581
43	6	0	-3.280072	-3.654967	0.609419
44	6	0	-3.112905	-2.340164	0.098022
45	6	0	-4.051869	-1.282556	0.201063
46	7	0	-3.475517	-0.025326	-0.008723
47	6	0	-5.427659	-1.384100	0.410692
48	6	0	-6.241477	-0.262860	0.281063
49	6	0	-4.306455	1.035541	-0.338625
50	6	0	-5.669057	0.954560	-0.154006
51	6	0	-3.571469	2.153126	-0.879230
52	6	0	-4.057713	3.468554	-1.001064
53	7	0	-2.289428	1.838104	-1.257610
54	6	0	-3.250199	4.449978	-1.531467
55	6	0	-1.510422	2.818516	-1.759074
56	6	0	-1.938369	4.117814	-1.924739
57	28	0	-1.768605	-0.027765	-0.761462
58	1	0	-0.055758	-2.600412	-1.169672
59	1	0	-0.292216	-4.929192	-0.383094
60	1	0	-2.414673	-5.593894	0.838027
61	1	0	-4.193439	-3.897797	1.144131
62	1	0	-5.867944	-2.356428	0.615941
63	1	0	-7.314568	-0.344906	0.410267
64	1	0	-6.302435	1.807237	-0.379786
65	1	0	-5.063815	3.696838	-0.665143
66	1	0	-3.616556	5.466105	-1.635089
67	1	0	-0.505963	2.520020	-2.043262
68	1	0	-1.271130	4.856982	-2.351960

Zero-point correction= 0.536662
(Hartree/Particle)
Thermal correction to Energy= 0.571036

Thermal correction to Enthalpy=	0.571980
Thermal correction to Gibbs Free Energy=	0.471277
Sum of electronic and zero-point Energies=	-1902.202286
Sum of electronic and thermal Energies=	-1902.167912
Sum of electronic and thermal Enthalpies=	-1902.166968
Sum of electronic and thermal Free Energies=	-1902.267672

Vt

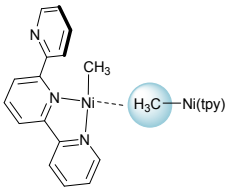


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.394236	1.063219	1.920361
2	6	0	-2.339155	0.361356	2.640308
3	6	0	-2.109515	-1.021316	2.856437
4	7	0	-0.261847	0.525721	1.435394
5	6	0	-0.950636	-1.590928	2.396273
6	6	0	0.007804	-0.800496	1.704405
7	6	0	1.297207	-1.262491	1.298960
8	7	0	2.165871	-0.294426	0.832796
9	6	0	1.708103	-2.617742	1.383139
10	6	0	2.988958	-2.967225	1.040226
11	6	0	3.449273	-0.647141	0.608177
12	6	0	3.899764	-1.955515	0.666898
13	6	0	4.450620	0.441204	0.424015
14	6	0	4.304188	1.651236	1.110718
15	7	0	5.510087	0.174050	-0.350459
16	6	0	5.283465	2.624567	0.966774
17	6	0	6.438239	1.122967	-0.485977
18	6	0	6.375013	2.363173	0.143189
19	28	0	1.078366	1.295338	0.083765
20	6	0	-0.128814	2.771382	-0.617191
21	6	0	2.342864	1.840996	-1.334748
22	1	0	-1.543389	2.114884	1.693573
23	1	0	-3.230720	0.857867	3.005345
24	1	0	-2.837782	-1.623272	3.391953
25	1	0	-0.753115	-2.642017	2.578416
26	1	0	1.000373	-3.376449	1.699719
27	1	0	3.307535	-4.004331	1.084955
28	1	0	4.943826	-2.165060	0.471929
29	1	0	3.428607	1.811263	1.730544
30	1	0	5.196477	3.573599	1.487297
31	1	0	7.279629	0.878398	-1.130825
32	1	0	7.161012	3.095119	-0.005620
33	1	0	0.607149	3.570732	-0.759318
34	1	0	-0.892651	3.149130	0.075125
35	1	0	-0.607147	2.692708	-1.618878
36	1	0	1.804968	2.102142	-2.257987
37	1	0	3.086009	1.069583	-1.577926
38	1	0	2.892688	2.738955	-1.016877
39	6	0	-3.553399	2.953544	-0.767535
40	6	0	-4.810043	3.450612	-0.434120

41	6	0	-5.768120	2.557887	0.031005
42	7	0	-3.227582	1.664622	-0.661034
43	6	0	-5.438913	1.211277	0.139115
44	6	0	-4.156702	0.795725	-0.217249
45	6	0	-3.735314	-0.633486	-0.154406
46	7	0	-2.537214	-0.879669	-0.683920
47	6	0	-4.497939	-1.658738	0.404222
48	6	0	-3.970509	-2.946598	0.395683
49	6	0	-2.013037	-2.107383	-0.694085
50	6	0	-2.718113	-3.186796	-0.158559
51	6	0	-0.653020	-2.195492	-1.291170
52	6	0	0.027673	-3.405164	-1.426334
53	7	0	-0.116111	-1.026860	-1.702236
54	6	0	1.301047	-3.405602	-1.983214
55	6	0	1.098510	-1.041683	-2.252138
56	6	0	1.850253	-2.203496	-2.412048
57	28	0	-1.285907	0.720681	-1.098177
58	1	0	-2.767766	3.611025	-1.128000
59	1	0	-5.022068	4.508042	-0.540147
60	1	0	-6.761473	2.900008	0.301698
61	1	0	-6.176284	0.497482	0.486381
62	1	0	-5.466884	-1.469469	0.850036
63	1	0	-4.536317	-3.765464	0.827664
64	1	0	-2.305171	-4.188221	-0.156023
65	1	0	-0.420402	-4.334208	-1.094047
66	1	0	1.852374	-4.335330	-2.080629
67	1	0	1.486912	-0.079071	-2.563161
68	1	0	2.839215	-2.151762	-2.852244

Zero-point correction= 0.535748
(Hartree/Particle)
Thermal correction to Energy= 0.570434
Thermal correction to Enthalpy= 0.571378
Thermal correction to Gibbs Free Energy= 0.470533
Sum of electronic and zero-point Energies= -1902.268741
Sum of electronic and thermal Energies= -1902.234055
Sum of electronic and thermal Enthalpies= -1902.233111
Sum of electronic and thermal Free Energies= -1902.333956

VIs



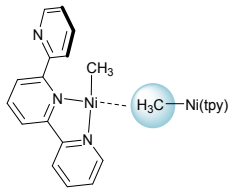
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.103676	-2.076845	-1.064538
2	6	0	-0.213353	-3.115265	-1.934377
3	6	0	0.765019	-3.567983	-2.809898
4	7	0	1.314597	-1.514327	-1.033309
5	6	0	2.026956	-2.981939	-2.781245
6	6	0	2.271852	-1.956312	-1.872542
7	6	0	3.603935	-1.318805	-1.701000
8	7	0	3.696731	-0.452419	-0.670642
9	6	0	4.703266	-1.629854	-2.495284
10	6	0	5.931874	-1.051361	-2.193855
11	6	0	4.900626	0.021414	-0.315273

12	6	0	6.041868	-0.239140	-1.075597
13	6	0	5.024199	0.756024	0.971400
14	6	0	4.260753	0.370444	2.075558
15	7	0	5.938342	1.730867	1.014039
16	6	0	4.432182	1.059692	3.270144
17	6	0	6.084828	2.388903	2.164163
18	6	0	5.354715	2.099395	3.315881
19	28	0	1.860792	0.272452	-0.156098
20	6	0	-0.181396	0.675378	0.537672
21	6	0	2.394734	2.102094	0.164881
22	1	0	-0.640651	-1.677067	-0.379897
23	1	0	-1.207911	-3.544962	-1.917658
24	1	0	0.556265	-4.371768	-3.507734
25	1	0	2.802345	-3.331120	-3.451452
26	1	0	4.610948	-2.308286	-3.333716
27	1	0	6.800535	-1.267577	-2.806360
28	1	0	6.987443	0.184913	-0.760480
29	1	0	3.555930	-0.450678	1.993181
30	1	0	3.856462	0.788001	4.148868
31	1	0	6.824147	3.186061	2.168187
32	1	0	5.519196	2.669059	4.223523
33	1	0	0.052838	1.584585	1.083122
34	1	0	0.134454	-0.241205	1.034377
35	1	0	-0.088307	0.738840	-0.557442
36	1	0	1.651021	2.760602	-0.300351
37	1	0	3.372397	2.312999	-0.284322
38	1	0	2.441914	2.333216	1.234904
39	6	0	-1.591687	-1.937593	2.200659
40	6	0	-1.846147	-3.145693	2.795979
41	6	0	-3.141867	-3.719936	2.636501
42	7	0	-2.493933	-1.229973	1.476110
43	6	0	-4.083424	-3.037363	1.920215
44	6	0	-3.780931	-1.767974	1.350046
45	6	0	-4.663795	-0.969406	0.599090
46	7	0	-4.010995	0.070409	-0.078281
47	6	0	-6.052865	-1.089410	0.487412
48	6	0	-6.791699	-0.117287	-0.173792
49	6	0	-4.765029	1.130110	-0.555816
50	6	0	-6.133519	1.042646	-0.658021
51	6	0	-3.947183	2.265707	-0.905912
52	6	0	-4.366395	3.380602	-1.656286
53	7	0	-2.648883	2.162019	-0.467081
54	6	0	-3.479436	4.399085	-1.924873
55	6	0	-1.794356	3.166673	-0.749377
56	6	0	-2.154638	4.294393	-1.454177
57	28	0	-2.239710	0.419935	0.407875
58	1	0	-0.615075	-1.475953	2.314604
59	1	0	-1.076293	-3.636469	3.379545
60	1	0	-3.372822	-4.686318	3.073894
61	1	0	-5.073968	-3.455723	1.767481
62	1	0	-6.559525	-1.922459	0.967854
63	1	0	-7.871226	-0.195356	-0.235656
64	1	0	-6.708973	1.867834	-1.066606
65	1	0	-5.387747	3.422833	-2.019694
66	1	0	-3.793858	5.266162	-2.496544
67	1	0	-0.782366	3.040035	-0.377526
68	1	0	-1.425049	5.074577	-1.636112

Zero-point correction= 0.535168
(Hartree/Particle)
Thermal correction to Energy= 0.570036

Thermal correction to Enthalpy=	0.570980
Thermal correction to Gibbs Free Energy=	0.467088
Sum of electronic and zero-point Energies=	-1902.190282
Sum of electronic and thermal Energies=	-1902.155414
Sum of electronic and thermal Enthalpies=	-1902.154470
Sum of electronic and thermal Free Energies=	-1902.258362

VIt

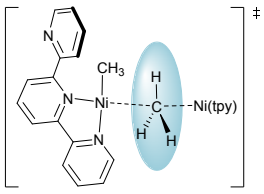


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.506061	1.008778	1.883151
2	6	0	-2.634994	0.333550	2.337804
3	6	0	-2.557542	-1.045139	2.498090
4	7	0	-0.357885	0.384208	1.606313
5	6	0	-1.368368	-1.699252	2.194565
6	6	0	-0.282142	-0.947393	1.742783
7	6	0	1.023093	-1.558227	1.363916
8	7	0	2.032977	-0.701255	1.123017
9	6	0	1.171475	-2.938665	1.231129
10	6	0	2.405675	-3.447613	0.844585
11	6	0	3.222595	-1.195324	0.752673
12	6	0	3.446672	-2.567344	0.598802
13	6	0	4.337385	-0.248005	0.469722
14	6	0	4.474703	0.953532	1.164504
15	7	0	5.195705	-0.643372	-0.481749
16	6	0	5.526370	1.799226	0.823119
17	6	0	6.199055	0.174584	-0.795167
18	6	0	6.403467	1.410242	-0.182201
19	28	0	1.373284	1.401508	1.012531
20	6	0	-1.543306	3.415223	-1.140698
21	6	0	2.214415	3.249195	0.661505
22	1	0	-1.510468	2.083289	1.723839
23	1	0	-3.551066	0.878295	2.541685
24	1	0	-3.416159	-1.610965	2.846646
25	1	0	-1.293937	-2.772472	2.321492
26	1	0	0.338208	-3.607679	1.407394
27	1	0	2.547491	-4.517772	0.733684
28	1	0	4.425123	-2.907727	0.283921
29	1	0	3.766741	1.222381	1.939671
30	1	0	5.653187	2.746734	1.336954
31	1	0	6.873765	-0.171453	-1.574678
32	1	0	7.233716	2.038980	-0.483784
33	1	0	-2.311489	3.932551	-1.745370
34	1	0	-1.657098	3.827274	-0.120728
35	1	0	-0.577348	3.809273	-1.499502
36	1	0	1.473630	4.015340	0.387614
37	1	0	2.918474	3.178484	-0.183339
38	1	0	2.789682	3.652040	1.511103
39	6	0	-4.695021	2.047187	-0.199721

40	6	0	-5.944165	1.833608	0.380211
41	6	0	-6.355034	0.521449	0.588921
42	7	0	-3.888055	1.050971	-0.555965
43	6	0	-5.511834	-0.522371	0.219053
44	6	0	-4.277398	-0.215580	-0.353166
45	6	0	-3.269759	-1.254273	-0.717562
46	7	0	-2.073595	-0.778558	-1.078775
47	6	0	-3.518652	-2.626575	-0.655132
48	6	0	-2.482933	-3.502045	-0.960631
49	6	0	-1.072334	-1.612658	-1.380693
50	6	0	-1.239004	-2.998109	-1.322192
51	6	0	0.214680	-0.951645	-1.744861
52	6	0	1.368754	-1.663205	-2.074880
53	7	0	0.196415	0.387998	-1.703152
54	6	0	2.535752	-0.954012	-2.343957
55	6	0	1.317203	1.064651	-1.954557
56	6	0	2.518182	0.434424	-2.275090
57	28	0	-1.733328	1.325349	-1.139886
58	1	0	-4.307399	3.046618	-0.382124
59	1	0	-6.568732	2.673841	0.660701
60	1	0	-7.318261	0.309186	1.041297
61	1	0	-5.811792	-1.549304	0.392371
62	1	0	-4.492803	-3.010439	-0.377414
63	1	0	-2.645098	-4.573920	-0.917413
64	1	0	-0.422834	-3.672162	-1.553391
65	1	0	1.371466	-2.746314	-2.111997
66	1	0	3.456786	-1.481136	-2.570971
67	1	0	1.238341	2.145719	-1.883315
68	1	0	3.414614	1.020135	-2.450394

Zero-point correction=	0.533906
(Hartree/Particle)	
Thermal correction to Energy=	0.570328
Thermal correction to Enthalpy=	0.571272
Thermal correction to Gibbs Free Energy=	0.465028
Sum of electronic and zero-point Energies=	-1902.283718
Sum of electronic and thermal Energies=	-1902.247296
Sum of electronic and thermal Enthalpies=	-1902.246352
Sum of electronic and thermal Free Energies=	-1902.352596

TS-2s



Imaginary frequency = -214.3429cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.146516	2.105709	-1.118552
2	6	0	0.147041	3.130834	-2.011883
3	6	0	-0.847625	3.554068	-2.883801
4	7	0	-1.349070	1.527198	-1.060543
5	6	0	-2.101030	2.952813	-2.827384
6	6	0	-2.321577	1.941314	-1.896350
7	6	0	-3.644065	1.290475	-1.700413

8	7	0	-3.715835	0.441244	-0.654736
9	6	0	-4.754191	1.573421	-2.490450
10	6	0	-5.972499	0.984854	-2.167575
11	6	0	-4.909941	-0.042961	-0.281428
12	6	0	-6.061659	0.190395	-1.034831
13	6	0	-5.012246	-0.763131	1.015341
14	6	0	-4.236247	-0.363452	2.105561
15	7	0	-5.921631	-1.741436	1.080046
16	6	0	-4.389347	-1.041594	3.308998
17	6	0	-6.050597	-2.388630	2.238334
18	6	0	-5.306743	-2.084595	3.377384
19	28	0	-1.860511	-0.258459	-0.150364
20	6	0	0.162723	-0.631259	0.485720
21	6	0	-2.369697	-2.093433	0.196996
22	1	0	0.611642	1.729914	-0.435601
23	1	0	1.136255	3.572928	-2.016925
24	1	0	-0.657913	4.345974	-3.600339
25	1	0	-2.889296	3.279369	-3.493908
26	1	0	-4.678393	2.236904	-3.342367
27	1	0	-6.849377	1.179273	-2.775789
28	1	0	-6.998652	-0.241047	-0.704587
29	1	0	-3.535199	0.458869	2.005723
30	1	0	-3.803327	-0.759216	4.177495
31	1	0	-6.786501	-3.188662	2.259996
32	1	0	-5.456432	-2.645768	4.292838
33	1	0	-0.024016	-1.542509	1.041568
34	1	0	-0.071652	0.301593	0.989358
35	1	0	0.151508	-0.683058	-0.608885
36	1	0	-1.632735	-2.753733	-0.276731
37	1	0	-3.355461	-2.317629	-0.228688
38	1	0	-2.393430	-2.317186	1.269677
39	6	0	1.619052	1.950270	2.199907
40	6	0	1.885702	3.150570	2.806816
41	6	0	3.186430	3.710996	2.656205
42	7	0	2.516839	1.239008	1.473972
43	6	0	4.123149	3.023018	1.937018
44	6	0	3.807143	1.762458	1.358226
45	6	0	4.687600	0.956677	0.606119
46	7	0	4.026371	-0.060458	-0.096043
47	6	0	6.077858	1.055050	0.524592
48	6	0	6.814805	0.076058	-0.133480
49	6	0	4.773939	-1.135212	-0.559806
50	6	0	6.146661	-1.067163	-0.634821
51	6	0	3.948779	-2.258258	-0.920740
52	6	0	4.360816	-3.373381	-1.677386
53	7	0	2.647907	-2.144599	-0.489066
54	6	0	3.465747	-4.380391	-1.957432
55	6	0	1.784844	-3.138462	-0.785543
56	6	0	2.138084	-4.265261	-1.494324
57	28	0	2.250839	-0.399273	0.382157
58	1	0	0.637048	1.498895	2.308073
59	1	0	1.119408	3.644980	3.391940
60	1	0	3.426962	4.671164	3.101879
61	1	0	5.118490	3.431368	1.789763
62	1	0	6.588146	1.873112	1.026242
63	1	0	7.896478	0.135419	-0.171972
64	1	0	6.715590	-1.901556	-1.034214
65	1	0	5.383332	-3.422594	-2.036816
66	1	0	3.774619	-5.246691	-2.533348
67	1	0	0.771121	-3.003785	-0.420927
68	1	0	1.402158	-5.037313	-1.685175

```
 ---------------------------------------------------------------------
 Zero-point correction=                           0.534529
(Hartree/Particle)
 Thermal correction to Energy=                    0.568945
 Thermal correction to Enthalpy=                  0.569889
 Thermal correction to Gibbs Free Energy=         0.466986
 Sum of electronic and zero-point Energies=          -1902.190885
 Sum of electronic and thermal Energies=             -1902.156469
 Sum of electronic and thermal Enthalpies=           -1902.155525
 Sum of electronic and thermal Free Energies=        -1902.258428
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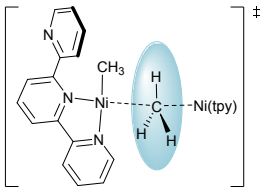
TS-2t



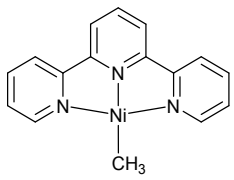
Imaginary frequency = -305.7761 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.427926	-2.147272	1.217206
2	6	0	0.224895	-3.389386	1.780981
3	6	0	1.354579	-4.224688	1.961150
4	7	0	1.625864	-1.688245	0.818143
5	6	0	2.593923	-3.772863	1.584621
6	6	0	2.737938	-2.481592	1.008303
7	6	0	3.980500	-1.907684	0.602603
8	7	0	3.929727	-0.582313	0.210048
9	6	0	5.210739	-2.613708	0.575657
10	6	0	6.365002	-1.968703	0.213491
11	6	0	5.095673	0.055753	-0.056784
12	6	0	6.317087	-0.584113	-0.082862
13	6	0	5.047806	1.535084	-0.218612
14	6	0	4.152960	2.297194	0.541852
15	7	0	5.929547	2.088601	-1.060813
16	6	0	4.159085	3.678045	0.399856
17	6	0	5.918122	3.416171	-1.192439
18	6	0	5.054345	4.256807	-0.495732
19	28	0	2.052602	-0.023982	-0.326920
20	6	0	-0.069528	0.607875	-0.423490
21	6	0	2.519839	1.031406	-1.933975
22	1	0	-0.411692	-1.473434	1.050932
23	1	0	-0.771239	-3.704343	2.068850
24	1	0	1.245173	-5.208885	2.406396
25	1	0	3.469146	-4.393154	1.744828
26	1	0	5.231482	-3.668264	0.828706
27	1	0	7.308227	-2.504609	0.180449
28	1	0	7.211458	-0.013556	-0.299791
29	1	0	3.475667	1.802655	1.230074
30	1	0	3.478950	4.293735	0.980711
31	1	0	6.639203	3.831359	-1.893103
32	1	0	5.092790	5.329855	-0.647029
33	1	0	0.153656	1.537740	-0.935651
34	1	0	0.055730	0.588742	0.660090
35	1	0	0.060683	-0.313708	-0.994809
36	1	0	1.790309	0.813372	-2.726781
37	1	0	3.522172	0.777451	-2.303543

38	1	0	2.492565	2.111796	-1.740087
39	6	0	-2.095945	3.451503	0.508265
40	6	0	-2.578637	4.682987	0.944035
41	6	0	-3.943785	4.810181	1.170412
42	7	0	-2.885922	2.400525	0.298539
43	6	0	-4.773494	3.713941	0.954238
44	6	0	-4.206859	2.519067	0.513815
45	6	0	-5.008338	1.286493	0.254617
46	7	0	-4.291774	0.212794	-0.091299
47	6	0	-6.398607	1.223116	0.353105
48	6	0	-7.025044	0.011809	0.081611
49	6	0	-4.880461	-0.957252	-0.350475
50	6	0	-6.267051	-1.097859	-0.275008
51	6	0	-3.948398	-2.061207	-0.726728
52	6	0	-4.379223	-3.371925	-0.921658
53	7	0	-2.656849	-1.710887	-0.866514
54	6	0	-3.447216	-4.341477	-1.279317
55	6	0	-1.771921	-2.643341	-1.215888
56	6	0	-2.116918	-3.975003	-1.434269
57	28	0	-2.225101	0.402509	-0.323187
58	1	0	-1.038295	3.289889	0.318346
59	1	0	-1.897782	5.511382	1.101067
60	1	0	-4.362644	5.749918	1.514662
61	1	0	-5.838846	3.796591	1.133008
62	1	0	-6.985844	2.091191	0.625612
63	1	0	-8.105090	-0.066606	0.144242
64	1	0	-6.753458	-2.039865	-0.495697
65	1	0	-5.420145	-3.642413	-0.791667
66	1	0	-3.761805	-5.368363	-1.433157
67	1	0	-0.742203	-2.311664	-1.318938
68	1	0	-1.356314	-4.695043	-1.712942

Zero-point correction= 0.532892
(Hartree/Particle)
Thermal correction to Energy= 0.568613
Thermal correction to Enthalpy= 0.569557
Thermal correction to Gibbs Free Energy= 0.460824
Sum of electronic and zero-point Energies= -1902.243289
Sum of electronic and thermal Energies= -1902.207568
Sum of electronic and thermal Enthalpies= -1902.206624
Sum of electronic and thermal Free Energies= -1902.315357

Ni(tpy)Me



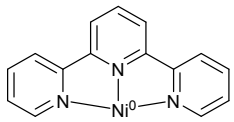
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.319158	0.044353	5.706655
2	6	0	0.023271	0.045697	4.662765
3	7	0	-0.744582	0.034016	1.982939
4	6	0	0.979509	-0.017440	3.668856
5	6	0	-1.331627	0.114538	4.305706
6	6	0	-1.660027	0.100653	2.962851
7	6	0	0.582270	-0.010614	2.323425
8	1	0	2.033914	-0.069968	3.916746

9	1	0	-2.112714	0.177471	5.053676
10	1	0	-2.692698	0.147503	2.635247
11	6	0	1.492806	-0.036004	1.190176
12	6	0	2.879127	0.000050	-1.214443
13	6	0	2.879127	0.000050	1.214443
14	7	0	0.829212	-0.080801	-0.000000
15	6	0	1.492806	-0.036004	-1.190176
16	6	0	3.579509	0.008067	-0.000000
17	1	0	3.418529	0.032212	2.155338
18	1	0	4.662781	0.040503	-0.000000
19	1	0	3.418529	0.032212	-2.155338
20	6	0	0.582270	-0.010614	-2.323425
21	6	0	-1.331627	0.114538	-4.305706
22	6	0	0.979509	-0.017440	-3.668856
23	7	0	-0.744582	0.034016	-1.982939
24	6	0	-1.660027	0.100653	-2.962851
25	6	0	0.023271	0.045697	-4.662765
26	1	0	2.033914	-0.069968	-3.916746
27	1	0	-2.692698	0.147503	-2.635247
28	1	0	0.319158	0.044353	-5.706655
29	1	0	-2.112714	0.177471	-5.053676
30	28	0	-1.085856	-0.047257	0.000000
31	6	0	-3.045969	-0.180672	0.000000
32	1	0	-3.424409	-0.717960	-0.879297
33	1	0	-3.507877	0.817927	0.000000
34	1	0	-3.424409	-0.717960	0.879297

Zero-point correction=	0.264440
(Hartree/Particle)	
Thermal correction to Energy=	0.280045
Thermal correction to Enthalpy=	0.280989
Thermal correction to Gibbs Free Energy=	0.221245
Sum of electronic and zero-point Energies=	-951.120485
Sum of electronic and thermal Energies=	-951.104880
Sum of electronic and thermal Enthalpies=	-951.103936
Sum of electronic and thermal Free Energies=	-951.163680

I.4. Atomic coordinates and energies for the stationary points in diisopropylether

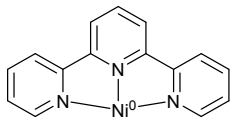
IVs



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

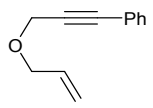
IVt



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000457	-0.258562	5.717467
2	6	0	0.000289	0.091154	4.689584
3	7	0	-0.000028	0.981768	2.050921
4	6	0	0.000135	-0.819152	3.649539
5	6	0	0.000289	1.461292	4.406458
6	6	0	0.000133	1.841627	3.070000
7	6	0	-0.000063	-0.364633	2.316418
8	1	0	0.000194	-1.883723	3.852418
9	1	0	0.000374	2.209275	5.189839
10	1	0	0.000183	2.893868	2.797741
11	6	0	-0.000256	-1.281740	1.179325
12	6	0	-0.000256	-2.713728	-1.222546
13	6	0	-0.000256	-2.713728	1.222546
14	7	0	-0.000340	-0.668880	-0.000000
15	6	0	-0.000256	-1.281740	-1.179325
16	6	0	-0.000276	-3.379806	-0.000000
17	1	0	-0.000298	-3.262232	2.155564
18	1	0	-0.000308	-4.467324	-0.000000
19	1	0	-0.000298	-3.262232	-2.155564
20	6	0	-0.000063	-0.364633	-2.316418
21	6	0	0.000289	1.461292	-4.406458
22	6	0	0.000135	-0.819152	-3.649539
23	7	0	-0.000028	0.981768	-2.050921
24	6	0	0.000133	1.841627	-3.070000
25	6	0	0.000289	0.091154	-4.689584
26	1	0	0.000194	-1.883723	-3.852418
27	1	0	0.000183	2.893868	-2.797741
28	1	0	0.000457	-0.258562	-5.717467
29	1	0	0.000374	2.209275	-5.189839
30	28	0	-0.000012	1.346731	0.000000

Zero-point correction= 0.232084
(Hartree/Particle)
Thermal correction to Energy= 0.246708
Thermal correction to Enthalpy= 0.247652
Thermal correction to Gibbs Free Energy= 0.189028
Sum of electronic and zero-point Energies= -911.275525
Sum of electronic and thermal Energies= -911.260902
Sum of electronic and thermal Enthalpies= -911.259957
Sum of electronic and thermal Free Energies= -911.318582

Enyne

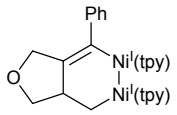


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.089725	-2.994722	1.188470
2	6	0	1.664579	-2.338326	0.077701
3	1	0	2.653612	-1.933794	0.339332
4	1	0	1.810673	-3.103183	-0.691084
5	6	0	1.360035	-2.361552	2.427811
6	1	0	2.446966	-2.304478	2.595609

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= (Hartree/Particle)	0.208267
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

VIIs



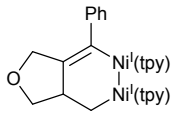
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.001065	5.571224	0.883237
2	6	0	-1.815372	4.502911	0.831552
3	7	0	-1.355838	1.746798	0.707274
4	6	0	-0.640121	3.978385	1.319613
5	6	0	-2.770921	3.635361	0.267854
6	6	0	-2.488034	2.285516	0.224246
7	6	0	-0.408063	2.591908	1.253097
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

VIIt

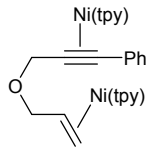


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.994536	5.225410	2.003385
2	6	0	-0.946785	4.161803	1.790124
3	7	0	-0.839631	1.424804	1.215479
4	6	0	0.176068	3.440863	2.110448
5	6	0	-2.036373	3.505094	1.171200
6	6	0	-1.922411	2.158614	0.899905
7	6	0	0.224554	2.053051	1.838157
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

VIIIs

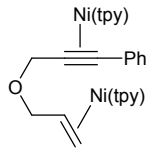


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.678714	-3.500491	-0.396175
2	6	0	0.878335	-2.276960	-1.099637
3	1	0	1.259037	-2.522726	-2.105063
4	1	0	1.655593	-1.687790	-0.597654
5	6	0	-0.336300	-1.439791	-1.239699
6	6	0	-1.635145	-1.372505	-1.198361
7	6	0	1.521131	-3.638361	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

VIIIt



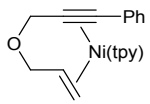
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.755588	-3.903127	-0.498296
2	6	0	0.172784	-3.003680	0.460233
3	1	0	0.013563	-3.575561	1.385107

4	1	0	-0.824771	-2.701313	0.105435
5	6	0	1.003419	-1.811604	0.747094
6	6	0	2.233646	-1.376114	0.684558
7	6	0	-0.011174	-4.058695	-1.658177
8	1	0	-1.044650	-4.339768	-1.404995
9	1	0	0.413591	-4.911561	-2.203102
10	6	0	0.014867	-2.860819	-2.585403
11	1	0	-0.759398	-2.821379	-3.352790
12	6	0	1.022659	-1.975862	-2.596981
13	1	0	1.105679	-1.217097	-3.370987
14	1	0	1.819935	-2.058371	-1.862247
15	28	0	1.053176	-0.007724	1.296148
16	1	0	-3.912118	-3.777954	1.738297
17	6	0	-3.145506	-3.134340	2.159823
18	7	0	-1.169654	-1.468364	3.224483
19	6	0	-3.030410	-1.812450	1.743254
20	6	0	-2.262749	-3.609016	3.122763
21	6	0	-1.297167	-2.733370	3.620820
22	6	0	-2.022729	-1.019346	2.295689
23	1	0	-3.702974	-1.397897	0.999357
24	1	0	-2.314297	-4.629570	3.485860
25	1	0	-0.592294	-3.067990	4.378264
26	6	0	-1.925465	0.426208	1.944728
27	6	0	-1.721798	3.136277	1.615151
28	6	0	-3.088802	1.196728	1.914746
29	7	0	-0.710579	0.963430	1.767795
30	6	0	-0.599036	2.298921	1.632027
31	6	0	-2.978011	2.572637	1.735963
32	1	0	-4.052826	0.726571	2.074557
33	1	0	-3.864323	3.198096	1.705158
34	1	0	-1.615545	4.205427	1.481264
35	6	0	0.784649	2.817973	1.563031
36	6	0	3.420370	3.596511	1.600592
37	6	0	1.094658	4.180269	1.577262
38	7	0	1.753253	1.878459	1.544524
39	6	0	3.031185	2.262946	1.568094
40	6	0	2.426906	4.570631	1.589386
41	1	0	0.309894	4.927159	1.591854
42	1	0	3.760084	1.460553	1.576710
43	1	0	2.684501	5.624915	1.605255
44	1	0	4.472357	3.855837	1.624332
45	28	0	-0.511400	-0.437794	-1.604538
46	1	0	-6.474111	-1.561848	-1.040652
47	6	0	-5.408855	-1.416207	-1.188106
48	7	0	-2.664885	-1.024012	-1.535859
49	6	0	-4.865841	-0.140092	-1.170898
50	6	0	-4.560089	-2.502218	-1.397956
51	6	0	-3.204859	-2.248076	-1.557151
52	6	0	-3.490549	0.032612	-1.369865
53	1	0	-5.502357	0.720234	-1.001180
54	1	0	-4.931287	-3.520107	-1.429927
55	1	0	-2.510484	-3.066705	-1.706240
56	6	0	-2.858091	1.374413	-1.422266
57	6	0	-1.484394	3.743666	-1.565462
58	6	0	-3.583600	2.551347	-1.469485
59	7	0	-1.517010	1.344886	-1.450368
60	6	0	-0.802633	2.510731	-1.541756
61	6	0	-2.863663	3.767115	-1.520835
62	1	0	-4.666582	2.556534	-1.476395
63	1	0	-3.395723	4.712342	-1.555309
64	1	0	-0.933804	4.676398	-1.632418

65	6	0	0.627503	2.353113	-1.649719
66	6	0	3.353746	1.900582	-1.833061
67	6	0	1.527296	3.448050	-1.680197
68	7	0	1.095549	1.069178	-1.717490
69	6	0	2.417199	0.880420	-1.796771
70	6	0	2.880280	3.223540	-1.773014
71	1	0	1.150062	4.462569	-1.615260
72	1	0	2.746486	-0.153679	-1.823182
73	1	0	3.571989	4.061003	-1.786939
74	1	0	4.410723	1.669522	-1.903173
75	1	0	7.112559	-3.066937	-0.809503
76	6	0	6.126722	-2.725878	-0.508085
77	6	0	3.558876	-1.842100	0.279923
78	6	0	5.096149	-3.642899	-0.299013
79	6	0	5.874782	-1.367138	-0.329367
80	6	0	4.610529	-0.936623	0.062650
81	6	0	3.831352	-3.209902	0.085334
82	1	0	5.280250	-4.704566	-0.440347
83	1	0	6.665508	-0.640005	-0.493716
84	1	0	4.408679	0.123294	0.181734
85	1	0	3.025609	-3.923207	0.227564

Zero-point correction= 0.671189
(Hartree/Particle)
Thermal correction to Energy= 0.714657
Thermal correction to Enthalpy= 0.715601
Thermal correction to Gibbs Free Energy= 0.594832
Sum of electronic and zero-point Energies= -2361.800377
Sum of electronic and thermal Energies= -2361.756910
Sum of electronic and thermal Enthalpies= -2361.755966
Sum of electronic and thermal Free Energies= -2361.876735

IXs

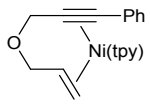


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.637111	0.757347	-0.330960
2	6	0	0.528850	3.583136	1.096053
3	1	0	-0.278600	4.278883	1.344981
4	1	0	1.190060	3.505114	1.976147
5	6	0	0.004206	2.233271	0.784110
6	6	0	-0.722663	1.220766	1.013800
7	6	0	2.232728	3.352481	-0.528436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

IXt

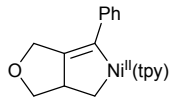


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.543233	0.820513	-0.441600
2	6	0	1.901108	2.906563	1.877549
3	1	0	1.690804	3.430644	2.814395
4	1	0	2.918119	2.489978	1.950206

5	6	0	0.945929	1.787618	1.737365
6	6	0	0.194274	0.836319	1.877576
7	6	0	2.360691	3.481601	-0.386418
8	1	0	3.236332	2.825057	-0.261805
9	1	0	2.704986	4.406747	-0.862700
10	6	0	1.325530	2.836330	-1.264621
11	1	0	0.373585	3.362225	-1.312558
12	6	0	1.573023	1.838662	-2.147581
13	1	0	0.849076	1.569701	-2.910561
14	1	0	2.550988	1.364382	-2.205064
15	1	0	4.741590	-3.587162	-0.274063
16	6	0	4.022299	-2.774437	-0.263948
17	7	0	2.172847	-0.704578	-0.261411
18	6	0	2.716611	-2.992909	-0.681708
19	6	0	4.393048	-1.503375	0.167208
20	6	0	3.428145	-0.504543	0.144822
21	6	0	1.802206	-1.935697	-0.663871
22	1	0	2.411020	-3.974621	-1.022482
23	1	0	5.399222	-1.288207	0.507890
24	1	0	3.665581	0.506809	0.468044
25	6	0	0.369227	-2.096313	-1.050090
26	6	0	-2.323198	-2.172006	-1.579909
27	6	0	-0.204068	-3.320569	-1.353455
28	7	0	-0.325889	-0.956706	-1.027401
29	6	0	-1.679702	-0.946700	-1.245189
30	6	0	-1.593334	-3.332109	-1.641603
31	1	0	0.365549	-4.240924	-1.359315
32	1	0	-2.082779	-4.268020	-1.893195
33	1	0	-3.389278	-2.195132	-1.779261
34	6	0	-2.332591	0.309614	-1.053711
35	6	0	-3.481196	2.765073	-0.400338
36	6	0	-3.743798	0.486573	-1.137736
37	7	0	-1.532339	1.379265	-0.696920
38	6	0	-2.117292	2.537574	-0.373874
39	6	0	-4.309852	1.692561	-0.813806
40	1	0	-4.373926	-0.343880	-1.438094
41	1	0	-1.436161	3.328384	-0.057926
42	1	0	-5.387164	1.820612	-0.867596
43	1	0	-3.887990	3.729417	-0.120914
44	1	0	-3.942172	-1.178821	2.126119
45	6	0	-2.863274	-1.288665	2.178171
46	6	0	-2.055123	-0.165901	2.036015
47	1	0	-2.493291	0.813366	1.866009
48	6	0	-0.661656	-0.302161	2.079440
49	6	0	-0.091158	-1.568544	2.277557
50	1	0	0.990600	-1.665187	2.301995
51	6	0	-0.906886	-2.683361	2.418347
52	1	0	-0.460370	-3.662397	2.561234
53	6	0	-2.294706	-2.546635	2.363334
54	1	0	-2.930330	-3.421216	2.461887
55	8	0	1.853450	3.888828	0.871943

Zero-point correction=	0.438406
(Hartree/Particle)	
Thermal correction to Energy=	0.466389
Thermal correction to Enthalpy=	0.467333
Thermal correction to Gibbs Free Energy=	0.378933
Sum of electronic and zero-point Energies=	-1450.497435
Sum of electronic and thermal Energies=	-1450.469453
Sum of electronic and thermal Enthalpies=	-1450.468509
Sum of electronic and thermal Free Energies=	-1450.556908

Xs

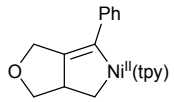


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.738942	5.164181	0.538967
2	6	0	-2.220968	4.210846	0.550160
3	7	0	-0.900498	1.772025	0.540799
4	6	0	-0.947948	4.102020	-0.001845
5	6	0	-2.802904	3.093452	1.132832
6	6	0	-2.107275	1.887924	1.096236
7	6	0	-0.306564	2.866801	0.029740
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

Xt

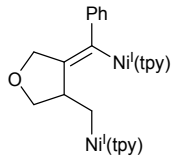


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.013717	5.933793	0.874607
2	6	0	-0.842414	4.880225	0.679946
3	7	0	-0.419158	2.193872	0.185580
4	6	0	-1.920432	4.031915	0.445647
5	6	0	0.448604	4.364461	0.661226
6	6	0	0.612150	3.004929	0.409231
7	6	0	-1.669408	2.683490	0.198264
8	1	0	-2.932042	4.419763	0.459385
9	1	0	1.312244	4.994688	0.838541
10	1	0	1.592498	2.534850	0.379683
11	6	0	-2.743374	1.681798	-0.064017
12	6	0	-4.525943	-0.353428	-0.563786
13	6	0	-4.106732	1.975484	-0.102189
14	7	0	-2.306345	0.436193	-0.266902
15	6	0	-3.148530	-0.570834	-0.512179
16	6	0	-4.998291	0.937886	-0.354836
17	1	0	-4.473817	2.982017	0.057570
18	1	0	-6.064105	1.136802	-0.390292
19	1	0	-5.218721	-1.162033	-0.762891
20	6	0	-2.493614	-1.895768	-0.712339
21	6	0	-1.102616	-4.238043	-1.034436
22	6	0	-3.201503	-3.073875	-0.944467
23	7	0	-1.152672	-1.884655	-0.644366
24	6	0	-0.473036	-3.018858	-0.798033
25	6	0	-2.491006	-4.259136	-1.108265
26	1	0	-4.283917	-3.076476	-0.993668
27	1	0	0.607959	-2.923602	-0.716610
28	1	0	-3.019977	-5.189001	-1.289443
29	1	0	-0.516164	-5.141791	-1.152826
30	28	0	-0.255473	0.004374	0.057392
31	1	0	0.068623	0.359005	2.638581
32	6	0	-0.208550	-0.539202	2.064535
33	1	0	-1.121384	-0.962925	2.505950
34	6	0	0.944627	-1.534714	2.073981
35	6	0	1.775329	-1.731756	3.343791
36	6	0	3.346075	-1.681044	1.668075

37	6	0	2.045504	-1.131230	1.100407
38	1	0	0.571069	-2.533222	1.783291
39	1	0	1.957691	-0.754830	3.824892
40	1	0	1.336018	-2.410313	4.080936
41	1	0	4.088244	-0.887802	1.843499
42	1	0	3.816451	-2.435086	1.024799
43	6	0	1.792523	-0.385953	0.012799
44	8	0	3.002639	-2.307518	2.904357
45	1	0	3.928352	1.179959	0.633788
46	1	0	5.668363	1.387289	-3.292887
47	6	0	4.897229	1.020088	-2.622663
48	6	0	2.877158	0.065287	-0.876690
49	6	0	3.877508	0.196876	-3.101181
50	6	0	4.905258	1.371073	-1.274040
51	6	0	3.914946	0.897765	-0.417033
52	6	0	2.880872	-0.260588	-2.245331
53	1	0	3.855233	-0.082754	-4.151360
54	1	0	5.688745	2.016863	-0.885896
55	1	0	2.077696	-0.886482	-2.630159

Zero-point correction=	0.441620
(Hartree/Particle)	
Thermal correction to Energy=	0.468287
Thermal correction to Enthalpy=	0.469231
Thermal correction to Gibbs Free Energy=	0.381368
Sum of electronic and zero-point Energies=	-1450.508876
Sum of electronic and thermal Energies=	-1450.482208
Sum of electronic and thermal Enthalpies=	-1450.481264
Sum of electronic and thermal Free Energies=	-1450.569127

XIs



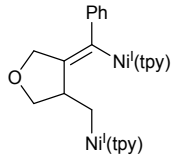
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.589470	-4.053268	3.914485
2	6	0	3.368490	-3.235091	3.237062
3	7	0	2.807911	-1.134720	1.502885
4	6	0	2.862954	-2.038071	3.726493
5	6	0	3.587296	-3.366975	1.866490
6	6	0	3.292674	-2.293087	1.038082
7	6	0	2.587949	-1.001273	2.838631
8	1	0	2.681520	-1.903835	4.786760
9	1	0	3.982362	-4.282176	1.441753
10	1	0	3.450332	-2.341340	-0.033994
11	6	0	2.030558	0.308822	3.233680
12	6	0	0.923939	2.817274	3.558105
13	6	0	1.648537	0.694278	4.501617
14	7	0	1.892568	1.128442	2.179137
15	6	0	1.323417	2.368944	2.280604
16	6	0	1.091784	1.992747	4.650704
17	1	0	1.753588	0.035682	5.355257
18	1	0	0.783833	2.331839	5.633919
19	1	0	0.481483	3.800705	3.679412

20	6	0	1.218374	3.033978	1.025101
21	6	0	1.144139	4.117637	-1.532052
22	6	0	0.671310	4.318062	0.824046
23	7	0	1.708929	2.305133	-0.060620
24	6	0	1.661169	2.858739	-1.280466
25	6	0	0.643882	4.865151	-0.438001
26	1	0	0.286338	4.871799	1.674523
27	1	0	2.053576	2.235835	-2.080063
28	1	0	0.242558	5.862677	-0.589152
29	1	0	1.142690	4.512437	-2.540465
30	28	0	2.306021	0.491510	0.430277
31	1	0	-0.152161	0.517460	0.224399
32	6	0	-0.453462	-0.327499	-0.410827
33	1	0	0.015352	-1.217437	0.035003
34	6	0	0.068120	-0.132946	-1.833555
35	6	0	-0.667246	-0.936895	-2.908139
36	6	0	1.495065	-1.135846	-3.527931
37	6	0	1.523902	-0.500296	-2.139599
38	1	0	-0.053724	0.924422	-2.121020
39	1	0	-0.828453	-1.977188	-2.568123
40	1	0	-1.632824	-0.509250	-3.194956
41	1	0	1.668479	-2.223579	-3.470399
42	1	0	2.227544	-0.715882	-4.225789
43	6	0	2.582883	-0.241124	-1.354156
44	1	0	7.065892	0.922406	-1.591929
45	1	0	-3.561713	-6.122174	0.583628
46	6	0	-3.302626	-5.081907	0.418109
47	7	0	-2.635926	-2.404875	0.000827
48	6	0	-4.284241	-4.101581	0.440115
49	6	0	-1.982135	-4.704834	0.176093
50	6	0	-1.698646	-3.361991	-0.024148
51	6	0	-3.929383	-2.772044	0.223863
52	1	0	-5.321121	-4.360297	0.621233
53	1	0	-1.181256	-5.433710	0.139784
54	1	0	-0.685655	-3.028304	-0.216207
55	6	0	-4.897149	-1.659223	0.187572
56	6	0	-6.392353	0.647371	-0.058181
57	6	0	-6.270430	-1.752112	0.304966
58	7	0	-4.295474	-0.474939	-0.014622
59	6	0	-4.991842	0.682855	-0.163301
60	6	0	-7.021607	-0.561803	0.183458
61	1	0	-6.765503	-2.701236	0.472226
62	1	0	-8.102274	-0.600115	0.266703
63	1	0	-6.977271	1.554121	-0.169878
64	6	0	-4.147529	1.813646	-0.441278
65	6	0	-2.357715	3.822178	-1.067380
66	6	0	-4.616822	3.119011	-0.660254
67	7	0	-2.791951	1.525389	-0.508966
68	6	0	-1.946751	2.527753	-0.793519
69	6	0	-3.732629	4.122914	-0.989629
70	1	0	-5.680606	3.321174	-0.588641
71	1	0	-0.891269	2.273830	-0.799916
72	1	0	-4.091716	5.127694	-1.186196
73	1	0	-1.626203	4.566296	-1.346458
74	28	0	-2.388247	-0.411273	-0.246340
75	8	0	0.188728	-0.912112	-4.038913
76	6	0	6.309929	0.182533	-1.840151
77	6	0	4.361155	-1.694030	-2.464095
78	6	0	6.669651	-0.980859	-2.520753
79	6	0	4.986897	0.396717	-1.469266
80	6	0	3.972374	-0.525492	-1.785627

81	6	0	5.687912	-1.920200	-2.824276
82	1	0	7.703254	-1.154958	-2.803761
83	1	0	4.713565	1.299436	-0.925740
84	1	0	5.954495	-2.836575	-3.343607
85	1	0	3.614757	-2.449839	-2.691441

Zero-point correction= 0.673871
(Hartree/Particle)
Thermal correction to Energy= 0.715233
Thermal correction to Enthalpy= 0.716177
Thermal correction to Gibbs Free Energy= 0.598579
Sum of electronic and zero-point Energies= -2361.781642
Sum of electronic and thermal Energies= -2361.740281
Sum of electronic and thermal Enthalpies= -2361.739337
Sum of electronic and thermal Free Energies= -2361.856934

XIt



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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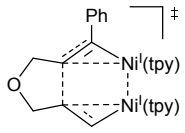
2	6	0	2.194123	-1.332453	4.715676
3	7	0	2.318005	-0.561670	2.056377
4	6	0	2.270208	0.013763	4.381196
5	6	0	2.178669	-2.286418	3.701625
6	6	0	2.240522	-1.855545	2.382484
7	6	0	2.331922	0.375544	3.038675
8	1	0	2.279989	0.778010	5.149961
9	1	0	2.120293	-3.345731	3.921397
10	1	0	2.226828	-2.547923	1.546669
11	6	0	2.410433	1.772048	2.549748
12	6	0	2.563587	4.203793	1.243954
13	6	0	2.445943	2.918834	3.310633
14	7	0	2.447299	1.820854	1.206761
15	6	0	2.526379	2.995050	0.509056
16	6	0	2.522819	4.160859	2.619735
17	1	0	2.416075	2.888861	4.393083
18	1	0	2.548492	5.084201	3.188324
19	1	0	2.622929	5.157485	0.728825
20	6	0	2.548195	2.793910	-0.904036
21	6	0	2.507766	2.145866	-3.601837
22	6	0	2.635775	3.819025	-1.876434
23	7	0	2.457931	1.467023	-1.301425
24	6	0	2.436077	1.183862	-2.616569
25	6	0	2.615058	3.500661	-3.211676
26	1	0	2.715591	4.852261	-1.552800
27	1	0	2.349720	0.127228	-2.854552
28	1	0	2.681081	4.283847	-3.960312
29	1	0	2.481994	1.856371	-4.645087
30	28	0	2.376252	0.202935	0.207302
31	1	0	-0.160674	-0.205179	0.702256
32	6	0	-0.768921	-0.912834	0.119265
33	1	0	-0.686229	-1.873393	0.651478

34	6	0	-0.178826	-1.084798	-1.285247
35	6	0	-1.074010	-1.923961	-2.212172
36	6	0	0.902798	-2.994093	-2.336871
37	6	0	1.149393	-1.840957	-1.376181
38	1	0	-0.040389	-0.093197	-1.744779
39	1	0	-1.630862	-2.672809	-1.620930
40	1	0	-1.793770	-1.333438	-2.786594
41	1	0	0.642765	-3.925700	-1.801218
42	1	0	1.747584	-3.206805	-2.999065
43	6	0	2.299261	-1.450451	-0.805966
44	1	0	6.888893	-1.683674	-1.484206
45	1	0	-5.980884	-5.003920	0.971464
46	6	0	-5.322514	-4.155508	0.816625
47	7	0	-3.636229	-1.974465	0.411447
48	6	0	-5.849405	-2.895656	0.572413
49	6	0	-3.939086	-4.309976	0.859521
50	6	0	-3.140509	-3.194500	0.652121
51	6	0	-4.986938	-1.818860	0.374547
52	1	0	-6.921500	-2.741706	0.533076
53	1	0	-3.480191	-5.273465	1.046445
54	1	0	-2.060124	-3.270852	0.674091
55	6	0	-5.442737	-0.438061	0.113624
56	6	0	-5.897582	2.237288	-0.390999
57	6	0	-6.746388	-0.002033	0.032939
58	7	0	-4.405912	0.404358	-0.046575
59	6	0	-4.580890	1.737056	-0.300127
60	6	0	-6.963535	1.378832	-0.226531
61	1	0	-7.583613	-0.677702	0.160232
62	1	0	-7.977760	1.756785	-0.295513
63	1	0	-6.072199	3.289827	-0.589138
64	6	0	-3.346536	2.441267	-0.440166
65	6	0	-0.848640	3.613593	-0.654463
66	6	0	-3.240381	3.826133	-0.701538
67	7	0	-2.206447	1.663339	-0.295914
68	6	0	-1.007218	2.265918	-0.405250
69	6	0	-2.003582	4.411018	-0.807802
70	1	0	-4.144666	4.415223	-0.813964
71	1	0	-0.138739	1.622720	-0.285561
72	1	0	-1.915698	5.474334	-1.007395
73	1	0	0.146618	4.032639	-0.731416
74	28	0	-2.606644	-0.253023	0.064249
75	8	0	-0.207109	-2.582636	-3.121195
76	6	0	5.966684	-2.233654	-1.318869
77	6	0	3.599200	-3.623515	-0.898069
78	6	0	5.988201	-3.627250	-1.257519
79	6	0	4.769650	-1.543345	-1.163401
80	6	0	3.551977	-2.220271	-0.966237
81	6	0	4.798305	-4.317881	-1.040912
82	1	0	6.923641	-4.166506	-1.370855
83	1	0	4.759834	-0.455648	-1.205594
84	1	0	4.802873	-5.402670	-0.980131
85	1	0	2.678749	-4.172357	-0.713606

Zero-point correction=	0.674341
(Hartree/Particle)	
Thermal correction to Energy=	0.715904
Thermal correction to Enthalpy=	0.716848
Thermal correction to Gibbs Free Energy=	0.596987
Sum of electronic and zero-point Energies=	-2361.816527
Sum of electronic and thermal Energies=	-2361.774964
Sum of electronic and thermal Enthalpies=	-2361.774020

Sum of electronic and thermal Free Energies= -2361.893881

TS-3s



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.417080	-3.609960	1.226684
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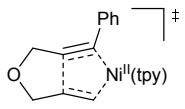
3	1	0	-2.272013	-3.486971	-0.793127
4	1	0	-0.708916	-3.567177	0.063042
5	6	0	-1.662486	-1.625744	0.124686
6	6	0	-2.645859	-0.755784	-0.159311
7	6	0	-1.798452	-3.031649	2.341560
8	1	0	-0.811269	-3.492280	2.507692
9	1	0	-2.421236	-3.250844	3.216632
10	6	0	-1.622461	-1.522918	2.234532
11	1	0	-2.557780	-0.970736	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

TS-4s



Imaginary frequency: -63.7139

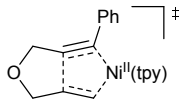
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.864337	3.980131	0.779464
2	6	0	3.058431	3.298972	1.033311

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-4t



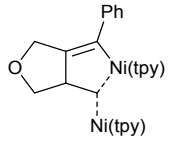
Imaginary frequency: -216.0509

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

TS-5s



Imaginary frequency = -288.9222

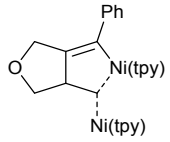
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	6.973054	2.796045	-1.538675
2	6	0	6.033114	2.276187	-1.386396
3	7	0	3.642981	0.952549	-0.980852
4	6	0	4.971952	2.923326	-0.760913
5	6	0	5.867899	0.970956	-1.835192
6	6	0	4.653435	0.337645	-1.599928
7	6	0	3.776756	2.231638	-0.590112
8	1	0	5.060871	3.955751	-0.444155
9	1	0	6.663305	0.440854	-2.344668
10	1	0	4.482402	-0.694071	-1.885779
11	6	0	2.534092	2.851884	-0.068854
12	6	0	0.140994	3.965209	0.610411
13	6	0	2.534343	4.002723	0.705143
14	7	0	1.397313	2.227904	-0.457277
15	6	0	0.217492	2.819646	-0.195940
16	6	0	1.304724	4.542527	1.084600
17	1	0	3.466005	4.457202	1.021059
18	1	0	1.266346	5.426264	1.712619
19	1	0	-0.836780	4.382210	0.816708
20	6	0	-1.004028	2.333929	-0.879340
21	6	0	-3.314400	1.747683	-2.216894
22	6	0	-0.923106	1.672555	-2.108557
23	7	0	-2.171079	2.655771	-0.303419
24	6	0	-3.290974	2.339856	-0.950742
25	6	0	-2.102174	1.390368	-2.791180
26	1	0	0.046114	1.420061	-2.528877
27	1	0	-4.221297	2.583182	-0.442532
28	1	0	-2.071697	0.872769	-3.746052
29	1	0	-4.257668	1.543198	-2.708805

30	28	0	1.931937	0.158215	-0.363635
31	1	0	0.209835	0.068059	1.063480
32	6	0	0.010675	-0.669260	0.281445
33	1	0	-0.093135	-0.310016	-0.744535
34	6	0	0.349301	-2.123951	0.542986
35	6	0	-0.094097	-2.720365	1.882864
36	6	0	1.973844	-3.672581	1.453457
37	6	0	1.818692	-2.411415	0.630931
38	1	0	-0.108618	-2.753892	-0.234840
39	1	0	0.122071	-2.018306	2.705496
40	1	0	-1.151281	-2.997595	1.922127
41	1	0	2.734369	-3.547346	2.238058
42	1	0	2.240697	-4.555851	0.861635
43	6	0	2.722969	-1.501113	0.249391
44	8	0	0.683808	-3.903873	2.025055
45	1	0	4.419380	0.080459	1.648685
46	1	0	7.969587	-2.293426	1.162667
47	6	0	6.910436	-2.137329	0.982895
48	6	0	4.162301	-1.725574	0.507169
49	6	0	6.180540	-3.061580	0.239777
50	6	0	6.268275	-1.010404	1.497610
51	6	0	4.914024	-0.807247	1.257968
52	6	0	4.821583	-2.857938	0.007064
53	1	0	6.669249	-3.943902	-0.163196
54	1	0	6.827197	-0.287871	2.085467
55	1	0	4.256452	-3.574253	-0.584295
56	1	0	-3.721988	1.381743	5.537364
57	6	0	-3.376498	0.997301	4.583546
58	7	0	-2.485286	-0.000356	2.126156
59	6	0	-4.276936	0.716211	3.572659
60	6	0	-2.012627	0.778277	4.349646
61	6	0	-1.623197	0.287906	3.117727
62	6	0	-3.816664	0.215234	2.351006
63	1	0	-5.339282	0.880259	3.714387
64	1	0	-1.266549	0.977972	5.109802
65	1	0	-0.576079	0.103734	2.907217
66	6	0	-4.668456	-0.108842	1.209305
67	6	0	-5.956698	-0.836985	-1.127107
68	6	0	-6.038554	-0.061216	1.177949
69	7	0	-3.933426	-0.439801	0.115262
70	6	0	-4.542165	-0.883011	-1.062957
71	6	0	-6.693964	-0.422042	-0.043978
72	1	0	-6.615568	0.232004	2.047543
73	1	0	-7.777242	-0.403256	-0.096691
74	1	0	-6.461213	-1.157242	-2.035120
75	6	0	-3.625051	-1.321636	-2.016741
76	6	0	-1.588112	-2.097234	-3.760214
77	6	0	-3.924469	-1.650372	-3.379149
78	7	0	-2.292432	-1.389065	-1.557272
79	6	0	-1.346325	-1.762020	-2.455752
80	6	0	-2.940507	-2.033144	-4.237102
81	1	0	-4.954478	-1.570087	-3.716196
82	1	0	-0.325853	-1.796123	-2.078603
83	1	0	-3.171683	-2.278013	-5.269538
84	1	0	-0.773416	-2.412263	-4.401109
85	28	0	-2.085890	-0.621824	0.243625

Zero-point correction= 0.673258
(Hartree/Particle)
Thermal correction to Energy= 0.714656
Thermal correction to Enthalpy= 0.715600

Thermal correction to Gibbs Free Energy= 0.599254
Sum of electronic and zero-point Energies= -2361.752280
Sum of electronic and thermal Energies= -2361.710882
Sum of electronic and thermal Enthalpies= -2361.709938
Sum of electronic and thermal Free Energies= -2361.826284

TS-5t



Imaginary frequency = -396.6574

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.077511	-4.140742	3.990038
2	6	0	3.010070	-3.295727	3.313177
3	7	0	2.825681	-1.134223	1.576912
4	6	0	2.419176	-2.110461	3.731984
5	6	0	3.508373	-3.382331	2.015658
6	6	0	3.390092	-2.279217	1.179033
7	6	0	2.347217	-1.041556	2.841715
8	1	0	2.011941	-2.019130	4.732329
9	1	0	3.980740	-4.286962	1.651162
10	1	0	3.756188	-2.294477	0.156952
11	6	0	1.744060	0.266619	3.174198
12	6	0	0.731297	2.818581	3.444928
13	6	0	1.293679	0.680420	4.424751
14	7	0	1.666931	1.089813	2.118417
15	6	0	1.198314	2.342541	2.221626
16	6	0	0.777987	1.969919	4.548455
17	1	0	1.348780	0.025712	5.286495
18	1	0	0.423034	2.318984	5.511768
19	1	0	0.347906	3.827192	3.543530
20	6	0	1.246388	3.085487	0.946167
21	6	0	1.410535	4.256673	-1.526653
22	6	0	0.690316	4.349602	0.760713
23	7	0	1.866297	2.423309	-0.061776
24	6	0	1.932572	2.994020	-1.268395
25	6	0	0.787094	4.947564	-0.490062
26	1	0	0.180648	4.852374	1.574707
27	1	0	2.419964	2.400538	-2.037118
28	1	0	0.369210	5.935087	-0.655464
29	1	0	1.497820	4.684499	-2.518390
30	28	0	2.209372	0.416589	0.382235
31	1	0	-0.379643	0.619303	0.303897
32	6	0	0.027878	-0.187574	-0.303865
33	1	0	0.190495	-1.156941	0.164651
34	6	0	0.306476	-0.008122	-1.774308
35	6	0	-0.515441	-0.776999	-2.821135
36	6	0	1.611958	-0.940569	-3.609683
37	6	0	1.718374	-0.400273	-2.194653
38	1	0	0.174812	1.059637	-2.024054
39	1	0	-0.651864	-1.826619	-2.504417
40	1	0	-1.496190	-0.338174	-3.026514
41	1	0	1.811374	-2.025415	-3.636225
42	1	0	2.283713	-0.458485	-4.329789

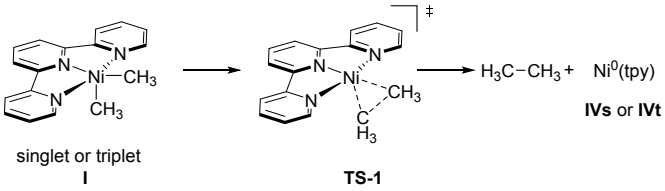
43	6	0	2.751680	-0.239490	-1.351508
44	1	0	7.279074	0.503148	-0.710110
45	1	0	-3.673593	-6.261671	0.176369
46	6	0	-3.367212	-5.222504	0.109783
47	7	0	-2.601851	-2.558784	-0.069225
48	6	0	-4.319796	-4.211723	0.116054
49	6	0	-2.021354	-4.883392	0.009960
50	6	0	-1.693605	-3.535469	-0.077890
51	6	0	-3.907625	-2.880229	0.024770
52	1	0	-5.373352	-4.455702	0.181779
53	1	0	-1.243660	-5.638622	-0.004704
54	1	0	-0.658360	-3.213346	-0.163995
55	6	0	-4.866022	-1.733840	0.007833
56	6	0	-6.420740	0.530949	-0.080840
57	6	0	-6.235251	-1.873523	0.159520
58	7	0	-4.277037	-0.548339	-0.174181
59	6	0	-5.007795	0.610714	-0.226872
60	6	0	-7.018294	-0.690299	0.110273
61	1	0	-6.705310	-2.836439	0.314573
62	1	0	-8.095987	-0.754395	0.225825
63	1	0	-7.028329	1.429318	-0.114371
64	6	0	-4.249854	1.806588	-0.432082
65	6	0	-2.630954	4.030556	-0.873285
66	6	0	-4.829579	3.100028	-0.559310
67	7	0	-2.876969	1.660232	-0.518475
68	6	0	-2.130681	2.747251	-0.735191
69	6	0	-4.033620	4.195804	-0.777355
70	1	0	-5.906268	3.217564	-0.491691
71	1	0	-1.055944	2.565293	-0.803013
72	1	0	-4.479807	5.180794	-0.881289
73	1	0	-1.968449	4.866864	-1.060799
74	28	0	-2.250232	-0.382461	-0.282467
75	8	0	0.266316	-0.708685	-4.009429
76	6	0	6.523142	-0.070949	-1.238507
77	6	0	4.572375	-1.530278	-2.577006
78	6	0	6.904758	-1.053407	-2.151257
79	6	0	5.175490	0.172298	-0.996383
80	6	0	4.162340	-0.538073	-1.667627
81	6	0	5.920947	-1.783914	-2.814456
82	1	0	7.955540	-1.251207	-2.339108
83	1	0	4.882340	0.933551	-0.275320
84	1	0	6.204345	-2.560107	-3.519936
85	1	0	3.824932	-2.125760	-3.091185

Zero-point correction= 0.671076
(Hartree/Particle)
Thermal correction to Energy= 0.713658
Thermal correction to Enthalpy= 0.714602
Thermal correction to Gibbs Free Energy= 0.591310
Sum of electronic and zero-point Energies= -2361.789513
Sum of electronic and thermal Energies= -2361.746932
Sum of electronic and thermal Enthalpies= -2361.745988
Sum of electronic and thermal Free Energies= -2361.869280

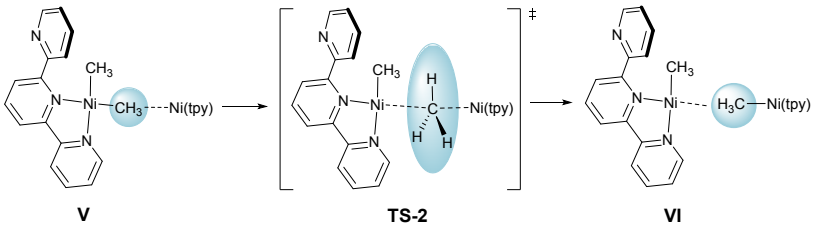
I.5. Energy comparison for key stationary points in solvent using M06-2X and M06 functionals

Calculations in THF

	G_{298} (u.a) - M06-2X	G_{298} (u.a) - M06
Is	-990.965986	-990.733086
I-bic	-990.980401	-990.749458
It	-990.997384	-990.733094
TS-1s	-990.915683	-990.709338
TS-1t	-990.970053	-990.727626
Ethane	-79.716996	-79.696299
IVs	-911.277032	-911.073855
IVt	-911.334861	-911.096409
Vt	-1902.333956	-1901.852359
TS-2t	-1902.315357	-1901.829623
VIt	-1902.352596	-1901.852611



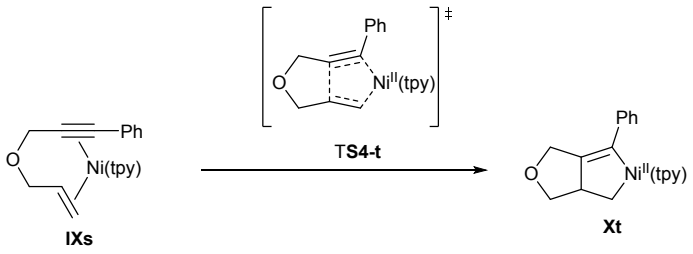
	I-bic Singlet **M06-2X**	**It** Triplet **M06-2X**	**I-bic** Singlet **M06**	**It** Triplet **M06**
ΔG_a	33.4	9.0	25.2	3.43
ΔG	-13.8	-39.1	-13.0	-37.4



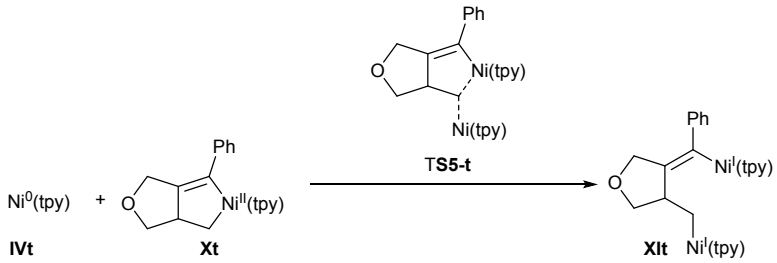
	Vt **M06-2X**	**Vt** **M06**
ΔG_a	15.7	14.3
ΔG	-7.3	-0.2

Calculations in diisopropylether

	G_{298} (u.a) - M06-2X	G_{298} (u.a) - M06
IXs	-1450.523794	-1450.119619
Xt	-1450.569127	-1450.161815
TS-4t	-1450.504877	-1450.102456
IVt	-911.318582	-911.098957
TS-5t	-2361.869280	-2361.248526
XIt	-2361.893881	-2361.285417



	M06-2X	M06
ΔG_a	11.9	10.8
ΔG	-28.5	-26.5



	M06-2X	M06
ΔG_a	11.6	7.7
ΔG	-3.9	-15.5