Transition Metal Intervention for a Classic Reaction—Assessing the Feasibility of Ni(0)-promoted [1,3] Sigmatropic Shifts of Bicyclo[3.2.0]hept-2-enes

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Supporting Information

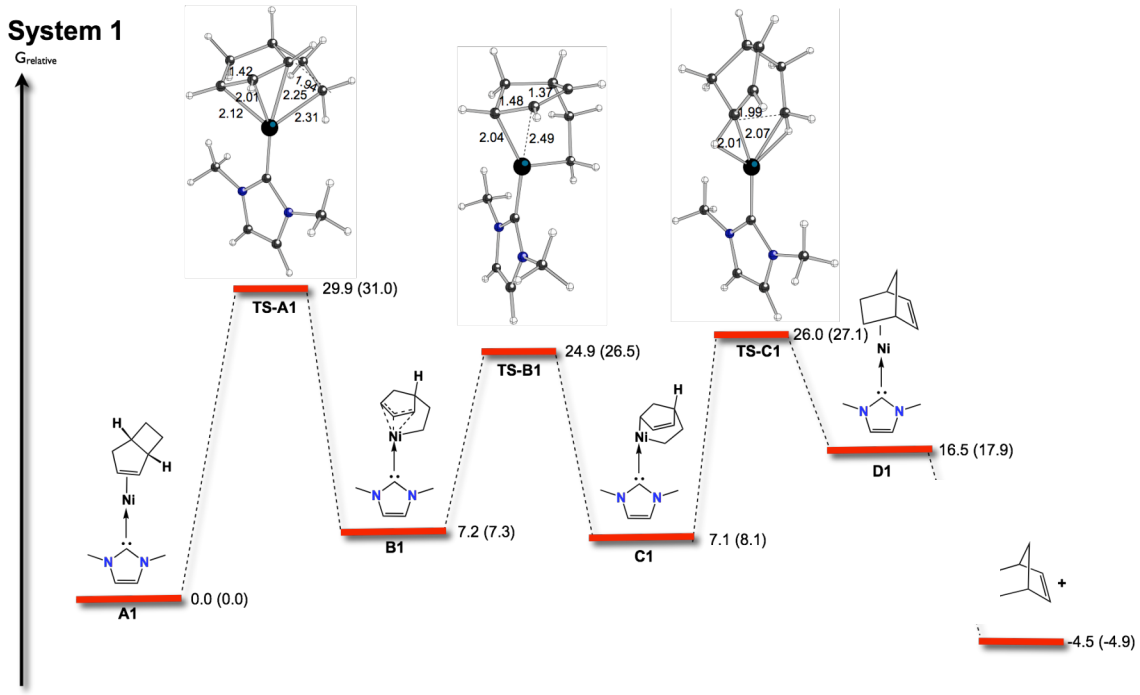
Full authorship of *Gaussian 03*:

Gaussian 03, Revision D.01,

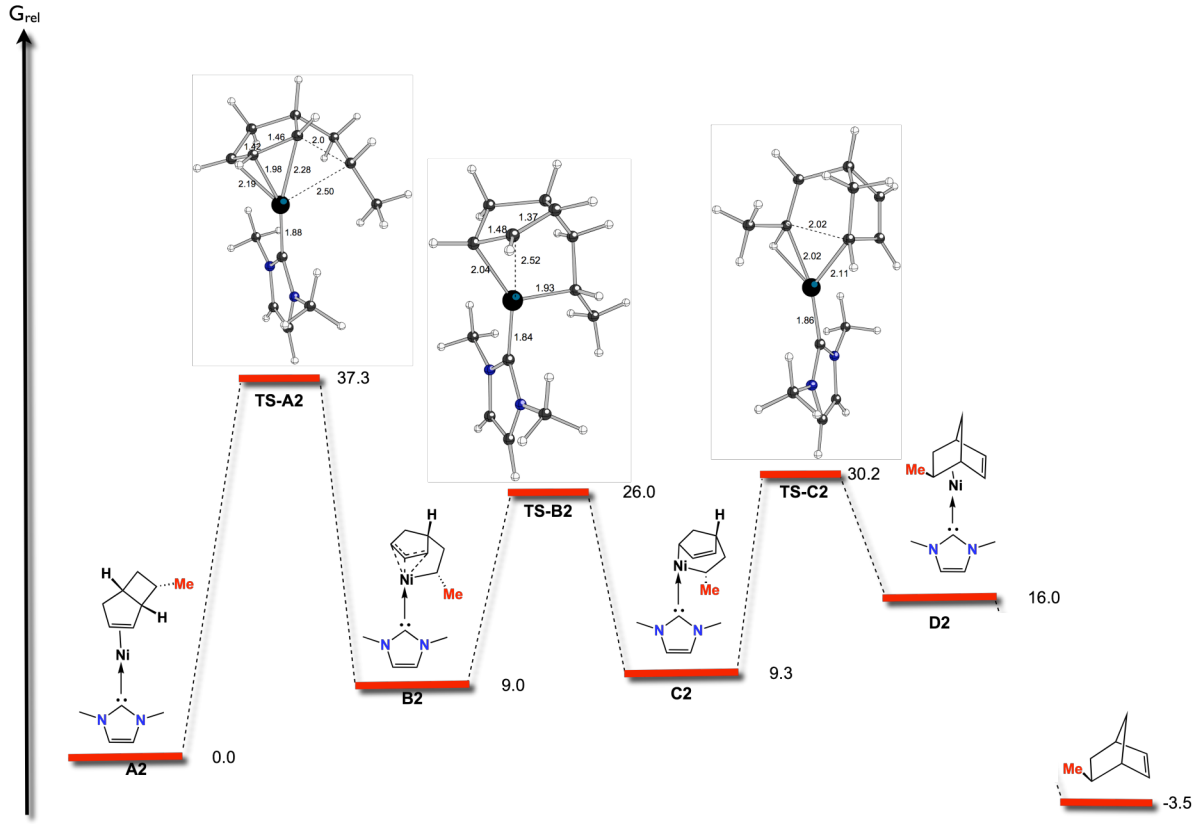
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004

Potential Energy Diagrams

Free energies at 298K shown in kcal/mol. The last energy in each case corresponds to the overall reaction energy from free reactant to free product.


System 1
Grelative
1.42
2.01
2.12
7.94
2.25
2.31
TS-A1
29.9 (31.0)
A1
0.0 (0.0)
B1
7.2 (7.3)
1.48
1.37
2.04
2.49
TS-B1
24.9 (26.5)
C1
7.1 (8.1)
1.99
2.07
2.01
TS-C1
26.0 (27.1)
D1
16.5 (17.9)
+
-4.5 (-4.9)

System 2



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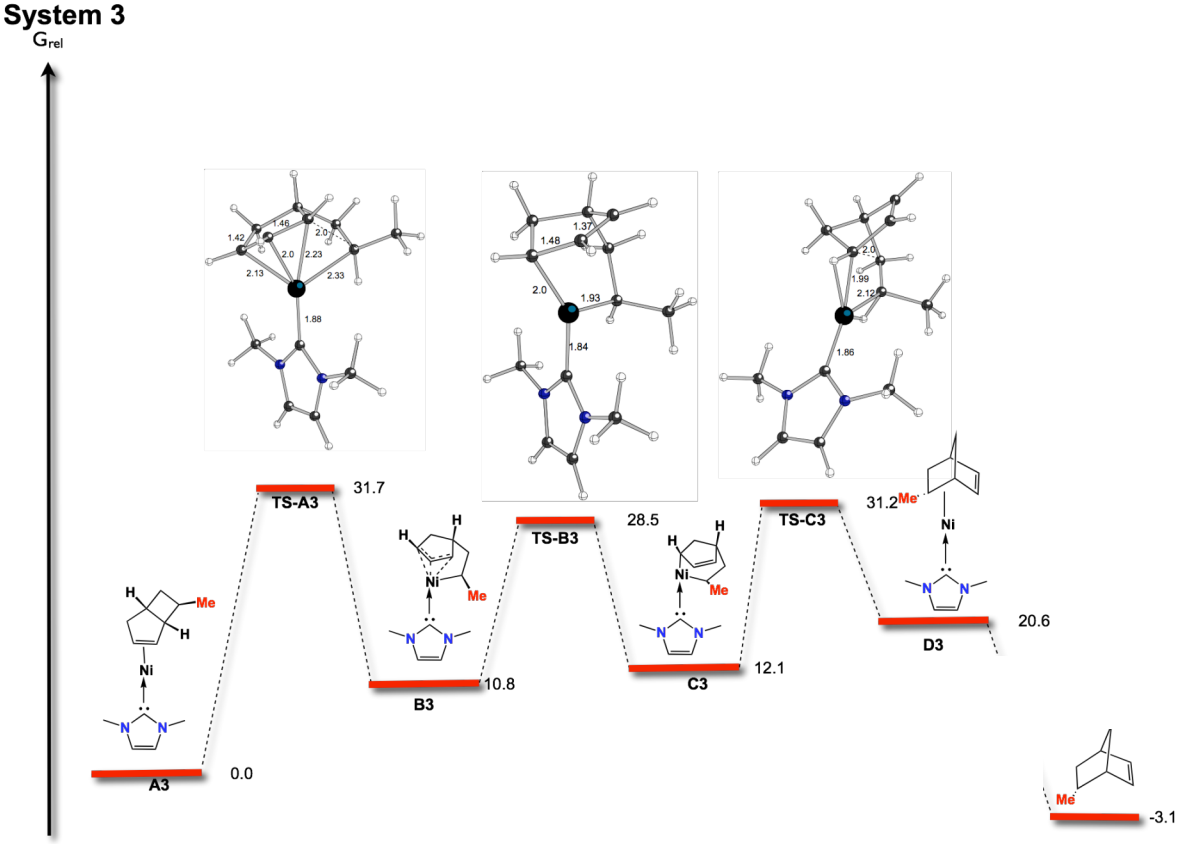

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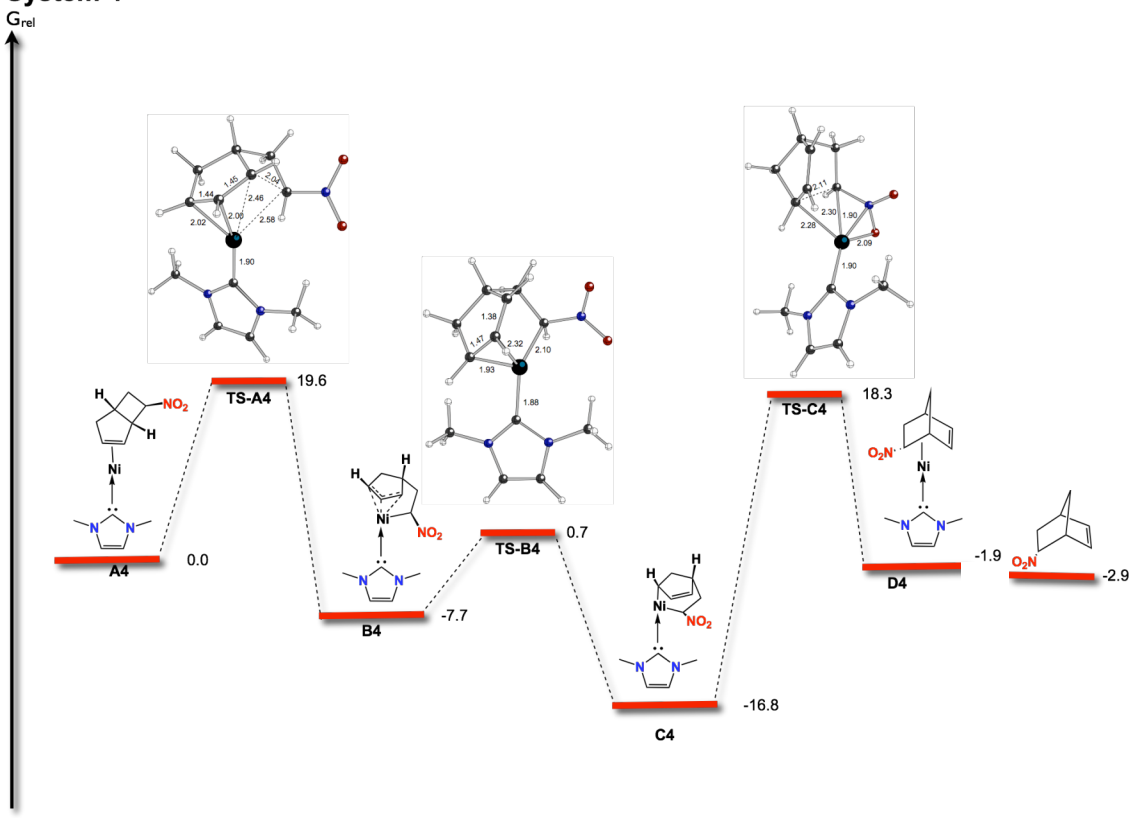

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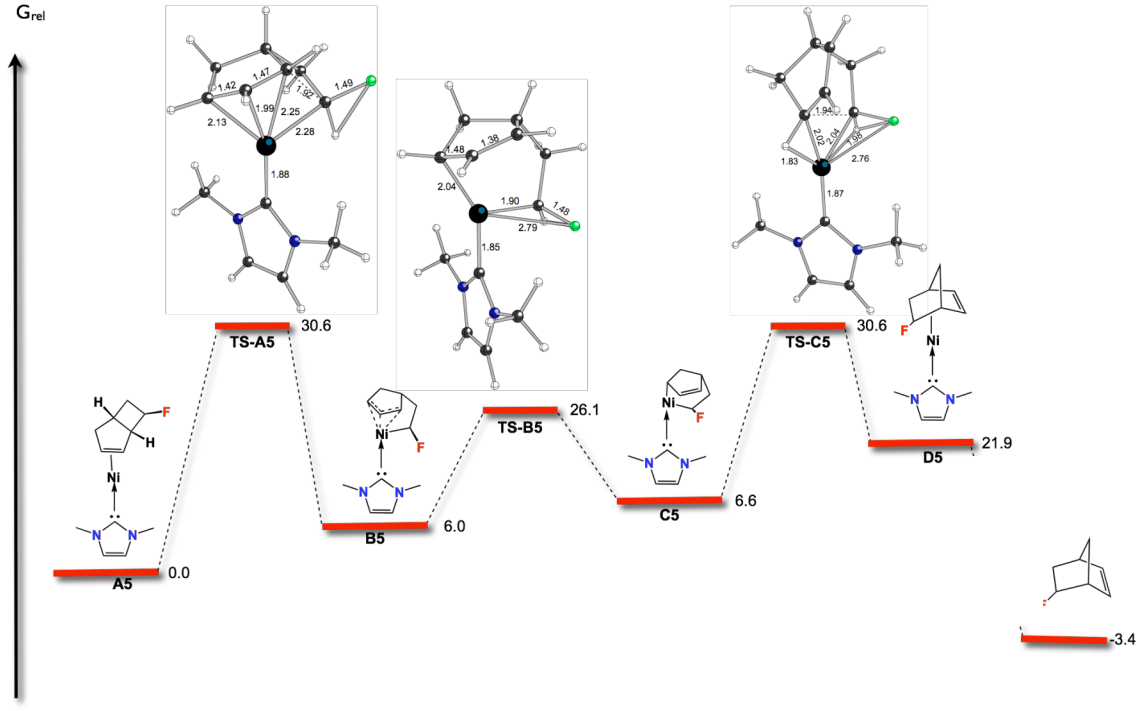
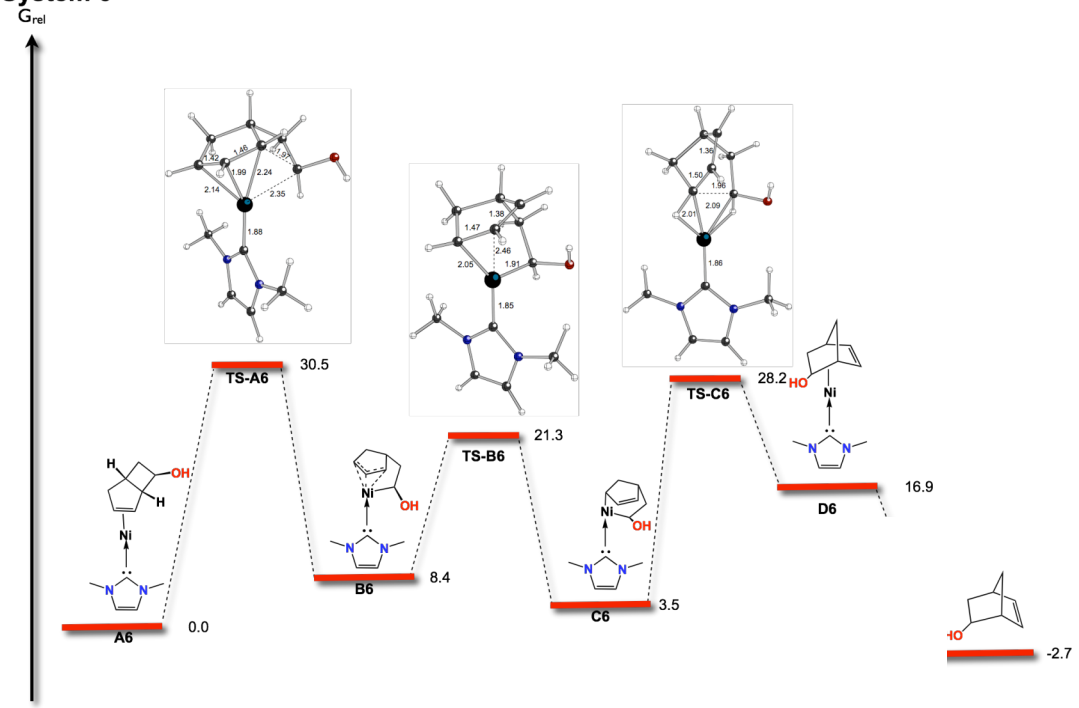
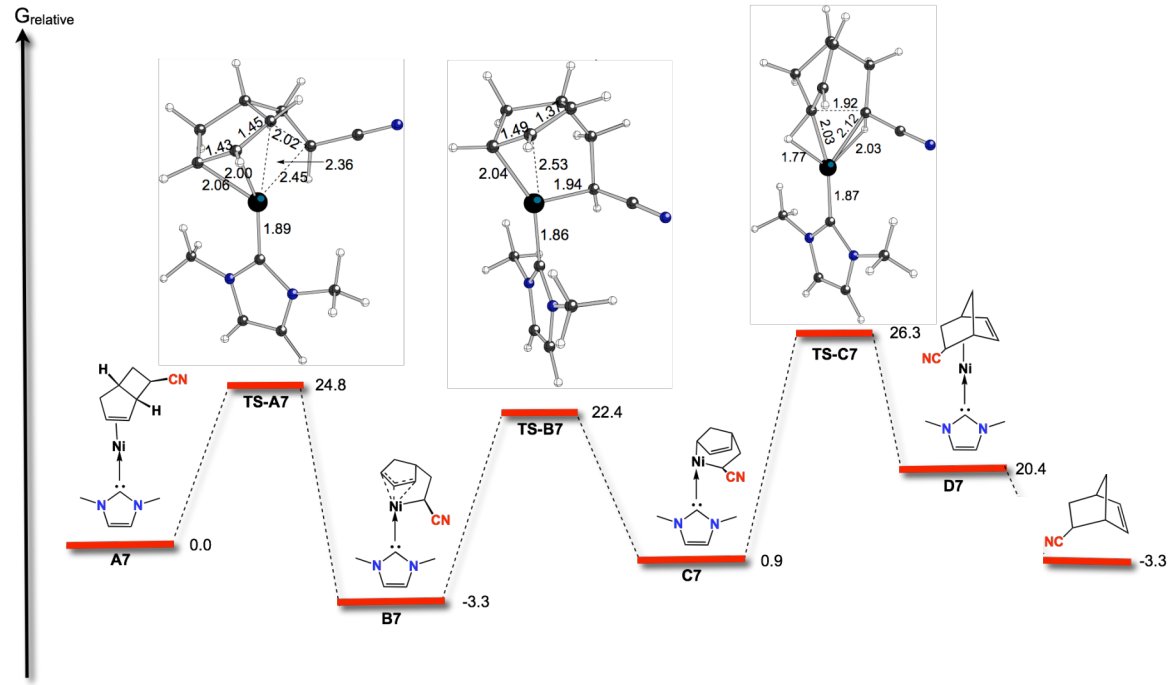


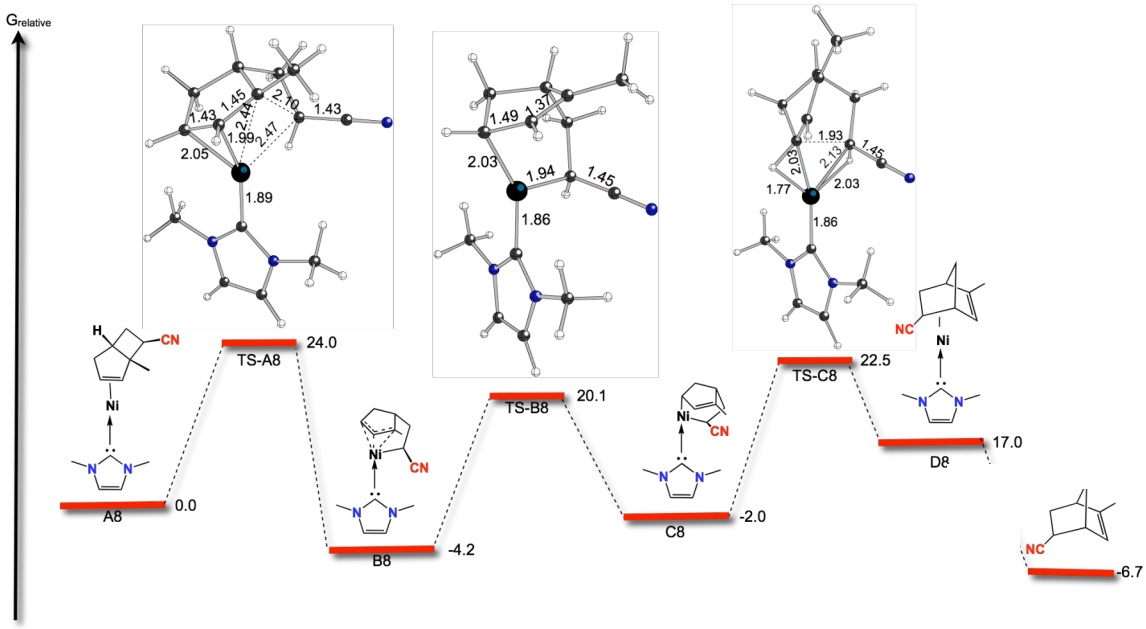
System 6



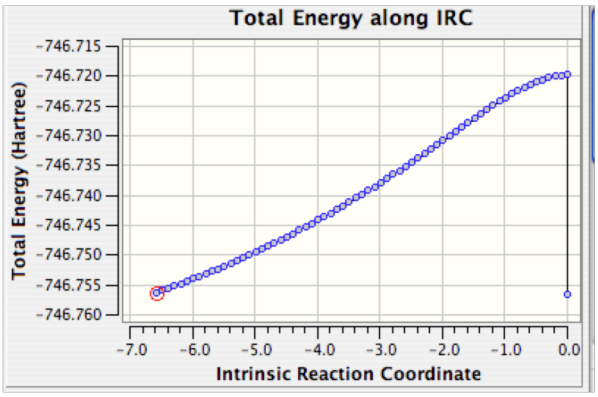
System 7



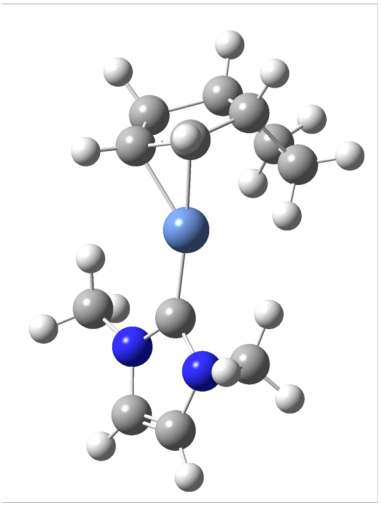
System 8



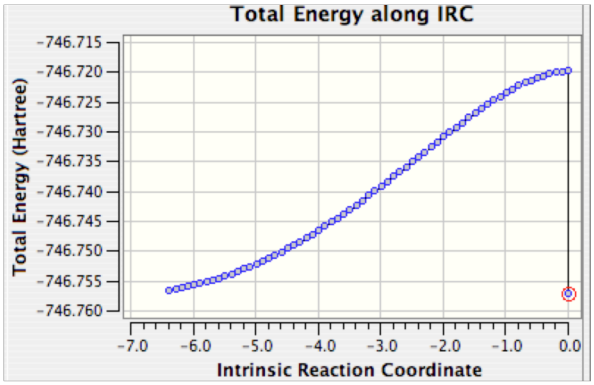
TS-A1 Reverse



Last structure



TS-A1 Forward



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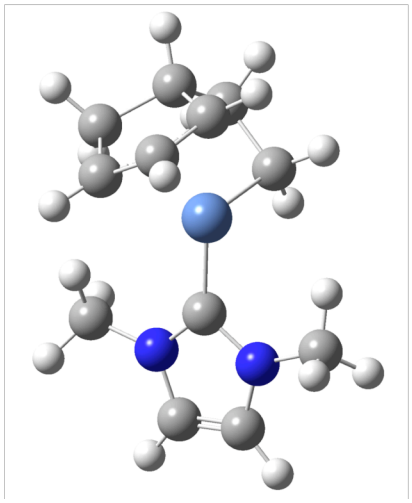
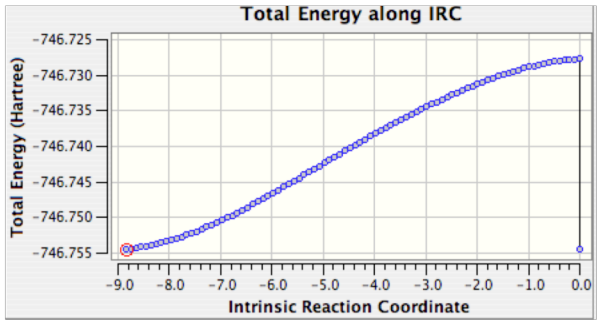


TS-B1 Reverse



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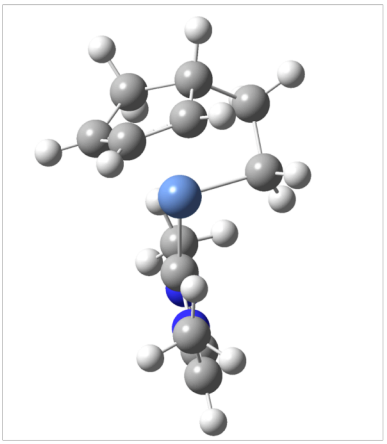
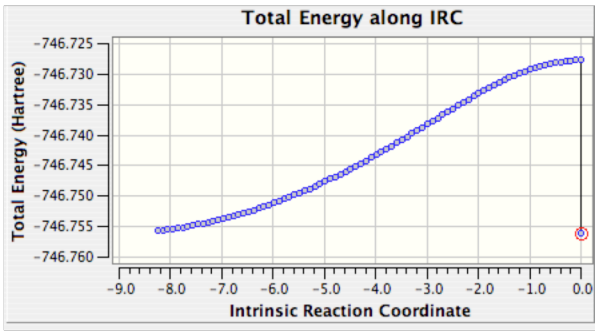
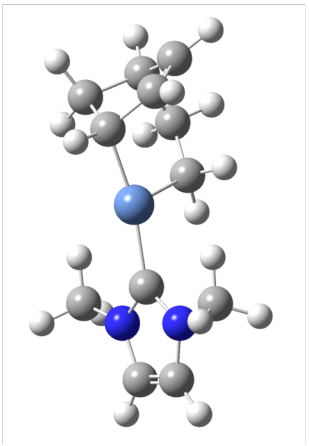


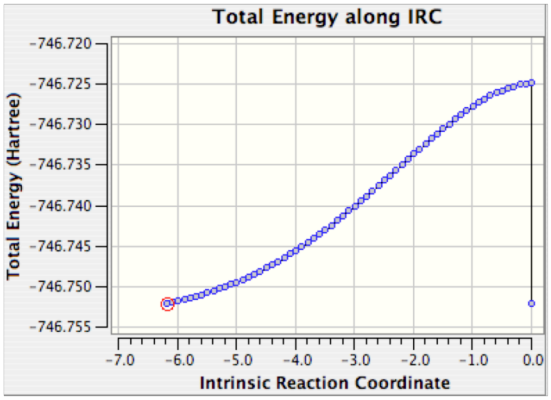
TS-B1 Forward



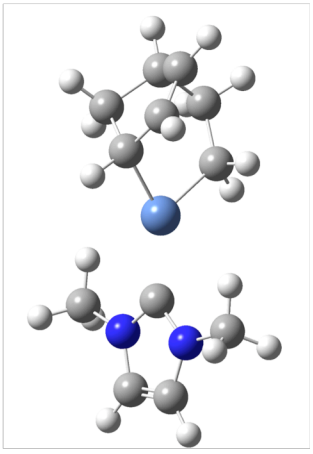
Last structure



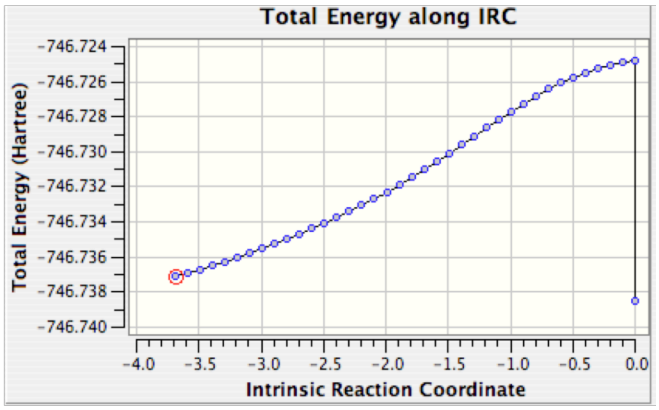
TS-C1 Reverse



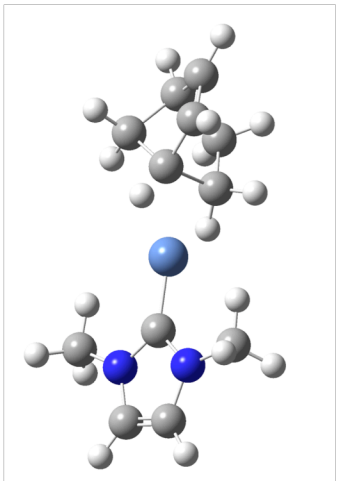
Last structure



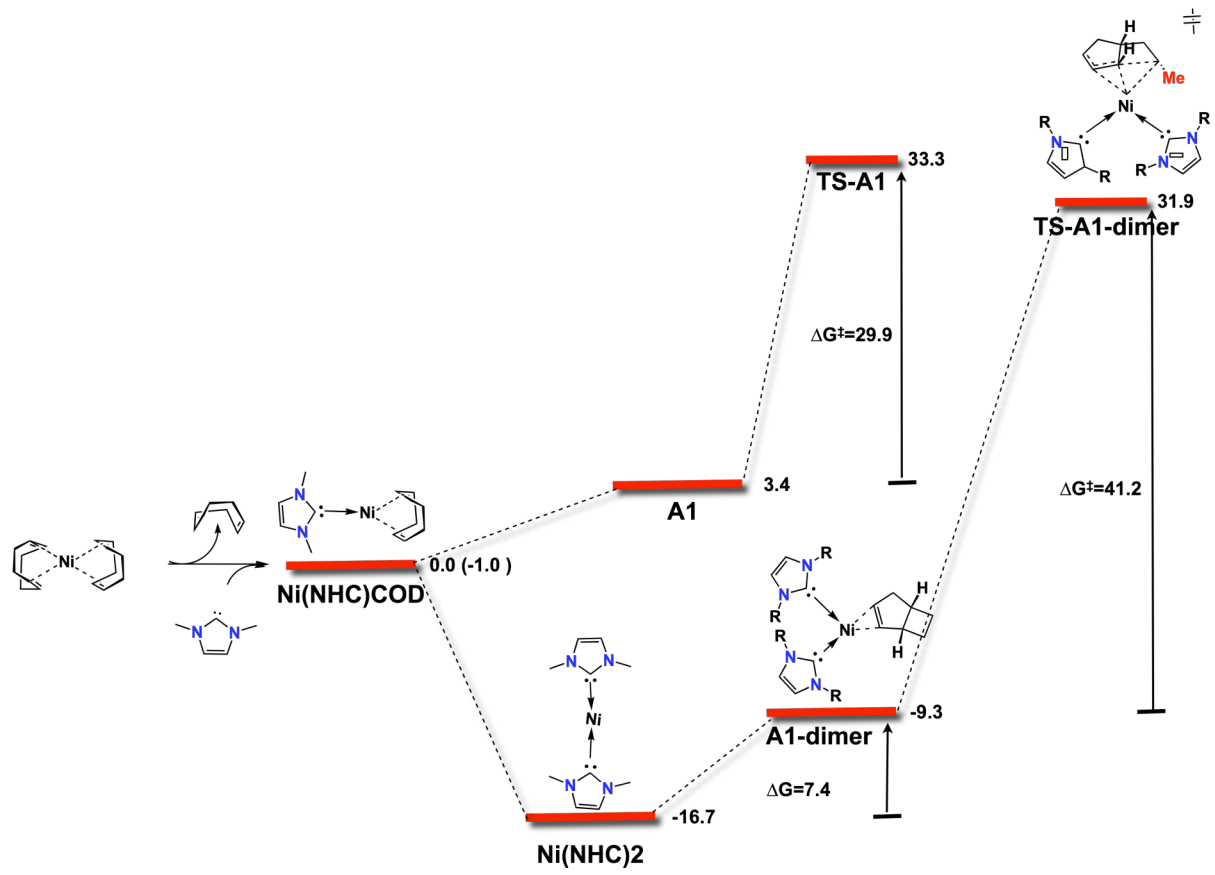
TS-C1 Forward



Last structure



SI-Figure 1. Resting catalytic state and comparison between oxidative transition states.



No imaginary frequencies found unless noted.
Energies in parenthesis computed using LANL2DZ for Ni and 6-31G(d) for all other atoms.

A1

E= -746.7674669
ZPE= 0.281454
H_{corr}= 0.298287
G_{corr}= 0.235563
E_{tot}= -746.469180
H_{tot}= -746.531904
G_{tot}= -746.531904 (

C	-2.88853	-0.44818	0.72564
C	-1.79384	-0.67694	-0.24088
C	-2.52867	0.02135	-1.60652
C	-3.70373	0.74646	-1.23456
C	-4.1341	0.30093	0.14443
H	-1.75145	-1.74918	-0.52138
H	-2.04438	0.20053	-2.57491
H	-4.23939	1.39714	-1.88421
H	-5.02206	-0.34942	0.0707
H	-4.42243	1.15351	0.77904
H	-3.18426	-1.3691	1.24859
C	-2.05405	0.43808	1.67732
H	-2.07494	1.47006	1.29205
H	-2.47044	0.47432	2.70189
C	-0.97932	-0.27228	1.0511
H	-0.89943	-1.29123	1.46769
H	-0.25331	0.38342	1.55818
Ni	-2.07746	1.95207	-1.27665
C	-0.75395	3.3964	-1.2798
C	1.02548	4.76856	-1.82142
C	0.529	5.19986	-0.61633
H	1.84956	5.13857	-2.41016
H	0.84881	6.00855	0.02115
N	-0.55004	4.36033	-0.30349
N	0.23653	3.6756	-2.21046
C	-1.36904	4.46472	0.9111
H	-2.09132	3.64523	0.89935
H	-0.74162	4.37847	1.80577
H	-1.90539	5.42064	0.93508
C	0.43255	2.89642	-3.43873
H	-0.23417	2.03136	-3.39697
H	0.19301	3.49637	-4.32477
H	1.46896	2.54681	-3.50842

TS-A1

E= -746.7197302
ZPE= 0.279499
H_{corr}= 0.295890
G_{corr}= 0.235476
E_{tot}= -746.440231
H_{tot}= -746.423841
G_{tot}= -746.484254 (

one imaginary frequency = -424.1 cm^{-1}

C	2.60411	-1.48428	0.01921
C	2.36443	-0.25004	-0.93675
C	1.68461	-0.90783	-2.13778
C	1.2233	-2.18937	-1.86013
C	2.04122	-2.74669	-0.68674
H	3.24736	0.20683	-1.405
H	1.67432	-0.39996	-3.10401
H	0.93369	-2.8449	-2.68406
H	2.85583	-3.38635	-1.06497
H	1.44401	-3.36604	0.00022
H	3.64233	-1.61546	0.34557
C	1.72388	-0.77523	1.10961
H	0.71234	-1.19611	1.15888
H	2.14517	-0.73181	2.12046
C	1.59425	0.79836	0.64761
H	2.30748	1.52587	1.0565
H	0.63426	1.29603	0.47264
Ni	0.22679	-0.20399	-0.80332
C	-1.6055	-0.05712	-0.333
C	-3.71599	0.7882	0.11575
C	-3.76088	-0.56163	0.3518
H	-4.48472	1.53899	0.20654
H	-4.57609	-1.1861	0.68094
N	-2.47776	-1.06236	0.07687
N	-2.40705	1.08148	-0.30086
C	-2.08746	-2.46943	0.19621
H	-1.02888	-2.54587	-0.06472
H	-2.23169	-2.82693	1.22326

H	-2.67164	-3.095	-0.48999
C	-1.92642	2.41807	-0.66042
H	-0.89786	2.32239	-1.01761
H	-2.5434	2.84841	-1.45866
H	-1.94207	3.08713	0.20899
C	2.63751	-1.08499	-0.25876
H	1.69166	-1.49916	0.10117
H	2.85874	-1.50098	-1.24955
H	3.4437	-1.35218	0.43371

B1

E= -746.7579023
ZPE=0.280426
H_{corr}= 0.296955
G_{corr}= 0.237467
E_{tot}= -746.477476
H_{tot}= -746.460947
G_{tot}= -746.520435 (

C	-2.83431	0.08793	0.62141
C	-2.48378	-0.81999	-0.5769
C	-2.25826	0.11418	-1.83555
C	-1.62057	1.16983	-1.22002
C	-2.29937	1.50206	0.13184
H	-2.84839	-1.8396	-0.64992
H	-2.12865	-0.19656	-2.86819
H	-1.09972	1.94243	-1.77894
H	-3.1217	2.23018	0.04641
H	-1.58246	1.91901	0.85397
H	-3.92041	0.14988	0.80314
C	-1.95451	-0.26887	1.86221
H	-1.70847	0.6463	2.42259
H	-2.52856	-0.90926	2.55473
C	-0.6448	-0.99662	1.3832
H	-0.76329	-2.0895	1.42439
H	0.22781	-0.72122	1.99404
Ni	-0.39773	0.09857	-0.31632
C	1.26119	1.01497	-0.39858
C	3.55739	1.28565	-0.331
C	3.00276	2.53697	-0.40755
H	4.59035	0.98026	-0.2863
H	3.46829	3.50903	-0.43075
N	1.60964	2.35775	-0.45521
N	2.49183	0.37285	-0.32159
C	0.63751	3.45108	-0.52022
H	-0.25423	3.09179	-1.03583
H	0.35616	3.78882	0.48491
H	1.06354	4.29417	-1.07476

TS-B1

E= -746.7276573
ZPE= 0.279330
H_{corr}= 0.295637
G_{corr}= 0.235445
E_{tot}= -746.448327
H_{tot}= -746.432020
G_{tot}= -746.492213 (

one imaginary frequency = -234.57 cm^{-1}

C	-2.83536	0.08829	0.61942
C	-2.48312	-0.82059	-0.57768
C	-2.06986	-0.04071	-1.70512
C	-1.67198	1.23767	-1.25826
C	-2.29997	1.50208	0.12938
H	-2.84736	-1.84037	-0.65025
H	-1.92124	-0.42218	-2.71115
H	-1.325	2.03398	-1.91099
H	-3.12225	2.23009	0.0425
H	-1.5839	1.91966	0.852
H	-3.9217	0.15026	0.79975
C	-1.87766	-0.46271	1.72399
H	-1.81113	0.25646	2.55494
H	-2.29671	-1.39027	2.15208
C	-0.37885	-0.82554	1.4136
H	-0.27097	-1.89668	1.18748
H	0.28785	-0.58181	2.25414
Ni	-0.08212	0.36705	-0.14532
C	1.49854	1.26274	0.40042
C	3.73224	1.51137	0.94732
C	3.10528	2.69163	1.25263
H	4.76625	1.22286	1.04665
H	3.4965	3.60409	1.67278
N	1.75218	2.52942	0.90916
N	2.74722	0.65264	0.43639
C	0.7233	3.55464	1.09622
H	-0.05079	3.41078	0.34106
H	0.26828	3.47958	2.09162
H	1.16538	4.54994	0.97903

C	2.98815	-0.7177	-0.02684
H	2.03159	-1.24735	-0.01231
H	3.38688	-0.72274	-1.04892
H	3.69744	-1.22027	0.64038

C1

E=-746.7566822
ZPE=0.280230
H_{corr}= 0.296792
G_{corr}=0.236029
E_{tot}= -746.476452
H_{tot}= -746.459890
G_{tot}= -746.520653 (

C	-4.03782	0.72418	0.11839
C	-4.39757	-0.58528	-0.59416
C	-3.23807	-1.15089	-1.01632
C	-1.9105	-0.17331	-0.92857
C	-2.79874	1.16647	-0.71702
H	-5.39571	-1.00786	-0.65135
H	-3.10056	-2.1227	-1.47963
H	-0.89061	-0.31346	-1.36422
H	-3.05046	1.4212	-1.75171
H	-2.22922	1.98356	-0.25792
H	-4.84792	1.44762	0.23715
C	-3.32441	0.32402	1.46785
H	-3.10906	1.22204	2.06045
H	-3.94017	-0.34608	2.07694
C	-1.92729	-0.33891	1.67322
H	-1.87977	-1.38978	1.97247
H	-1.046	0.1845	2.13117
Ni	-0.48827	-0.1986	0.30108
C	1.31642	-0.07257	0.22399
C	3.57891	-0.60481	0.16111
C	3.4831	0.76076	0.09451
H	4.44826	-1.24316	0.15995
H	4.25493	1.51079	0.02393
N	2.11517	1.07547	0.134
N	2.26776	-1.10168	0.23851
C	1.57103	2.43134	0.07738
H	0.48497	2.35303	0.17869
H	1.96684	3.04636	0.89595
H	1.80762	2.91127	-0.88132
C	1.91771	-2.51841	0.32794
H	0.82621	-2.58679	0.32715
H	2.31448	-3.07451	-0.53131
H	2.30445	-2.96249	1.25458

TS-C1

E= -746.7247924
ZPE= 0.279320
H_{corr}= 0.295659
G_{corr}= 0.234349
E_{tot}= -746.445472
H_{tot}= -746.429133
G_{tot}= -746.490443 (

one imaginary frequency = -365.62 cm^{-1}

C	3.39773	-0.70107	0.36252
C	3.62907	0.78845	0.61397
C	2.81026	1.50863	-0.20612
C	1.88264	0.54836	-0.97527
C	2.87499	-0.68315	-1.10327
H	4.25573	1.18241	1.40968
H	2.69605	2.5912	-0.18944
H	1.51631	0.94648	-1.94755
H	3.72426	-0.58051	-1.80069
H	2.3202	-1.595	-1.36453
H	4.29716	-1.31861	0.49245
C	2.25771	-1.25789	1.28848
H	2.05902	-2.30016	0.98955
H	2.64734	-1.29762	2.32055
C	1.19475	-0.14024	0.5626
H	1.28267	0.80272	1.12568
H	0.30609	-0.69105	0.90936
Ni	-0.38127	0.37226	-0.77009
C	-2.31859	0.17789	-0.48835
C	-4.54121	0.62648	-0.03368
C	-4.43	-0.72745	-0.23031
H	-5.40336	1.22982	0.20169
H	-5.17931	-1.50203	-0.19459
N	-3.07851	-0.9825	-0.50748
N	-3.25353	1.16067	-0.19397
C	-2.51611	-2.31051	-0.78125
H	-1.43859	-2.19473	-0.91759
H	-2.70231	-2.98821	0.05998
H	-2.95352	-2.73512	-1.69263
C	-2.91334	2.58115	-0.05014

H	-1.82561	2.67334	-0.10469
H	-3.36806	3.17472	-0.85217
H	-3.25566	2.96048	0.91954

D1

E= -746.7406652
ZPE= 0.281967
H_{corr}= 0.298887
G_{corr}= 0.235071
E_{tot}= -746.458699
H_{tot}= -746.441778
G_{tot}= -746.505594 (

C	-2.87902	-0.27928	-0.57268
C	-1.69112	-1.11514	-1.16745
C	-0.59547	-0.11151	-1.36204
C	-1.25152	0.67464	-0.18026
C	-2.47946	1.22505	-0.74689
H	-1.93542	-1.67449	-2.08798
H	0.40162	-0.38033	-1.70648
H	-0.62755	1.56108	-0.27813
H	-3.05034	1.72379	-1.54772
H	-2.66271	1.79984	0.17327
H	-3.81242	-0.50441	-1.10913
C	-3.02279	-0.71068	0.90121
H	-3.70386	-0.00484	1.40339
H	-3.47844	-1.71377	0.99217
C	-1.5199	-0.25236	1.07076
H	-0.84465	-1.03765	0.68053
H	-1.53733	-0.33569	2.17621
Ni	-0.65412	1.37719	1.61151
C	-0.15423	1.91707	3.44517
C	1.0418	2.41554	5.35959
C	-0.28999	2.5548	5.66287
H	1.91659	2.55932	5.97336
H	-0.77003	2.83799	6.58591
N	-1.00087	2.24795	4.49334
N	1.10667	2.02634	4.01342
C	-2.46453	2.26828	4.37071
H	-2.71494	2.1357	3.31557
H	-2.91383	1.45689	4.9555
H	-2.86358	3.22849	4.7164
C	2.35018	1.77576	3.27448
H	2.08317	1.51739	2.247
H	2.98194	2.67163	3.26833
H	2.90593	0.94412	3.72325

1

E= -272.7173537
ZPE= 0.152225
H_{corr}= 0.158930
G_{corr}=0.122823
E_{tot}= -272.565129
H_{tot}= -272.558424
G_{tot}= -272.594531

C	-0.18783	-0.80949	0.57258
C	-0.3781	0.7581	0.63845
C	0.85414	1.28263	-0.07204
C	1.72819	0.29949	-0.3872
C	1.25617	-1.07851	0.06872
H	-0.52543	1.22079	1.62262
H	0.99869	2.33779	-0.29411
H	2.67575	0.45146	-0.89981
H	1.90982	-1.47509	0.86103
H	1.27134	-1.81468	-0.74939
H	-0.42464	-1.34962	1.49504
C	-1.33823	-0.87747	-0.49571
H	-0.96272	-1.0677	-1.50788
H	-2.14394	-1.5887	-0.28452
C	-1.68006	0.63201	-0.23626
H	-2.59827	0.76949	0.34726
H	-1.72619	1.27559	-1.12146

2

E= -272.6820283
ZPE= 0.153826
H_{corr}= 0.159956
G_{corr}= 0.125297
E_{tot}= -272.528202
H_{tot}= -272.522072
G_{tot}= -272.556731

C	-2.96864	-1.11134	0.0205
C	-1.94776	-0.68979	-1.0663
C	-1.88665	0.73172	-1.01562
C	-2.86889	1.1613	0.10334
C	-3.98504	0.07692	-0.08313
H	-1.78724	-1.30468	-1.9527
H	-1.67377	1.39333	-1.85604
H	-3.18791	2.20719	0.05383
H	-4.4767	0.13392	-1.06089
H	-4.74222	0.08217	0.71461
H	-3.37768	-2.11893	-0.10368
C	-2.37241	-0.8379	1.44498
H	-3.03659	-1.23604	2.2248
H	-1.38663	-1.29968	1.56617
C	-2.30362	0.73412	1.50214
H	-1.28196	1.09813	1.65404
H	-2.9344	1.13082	2.30985
C	3.78847	-0.69974	0.36787
C	3.76353	0.63974	0.5806
H	4.58918	-1.41632	0.47139
H	4.5398	1.31835	0.90032
N	2.47137	1.06194	0.29911
N	2.51242	-1.05943	-0.04341
C	2.01817	2.44096	0.39016
H	0.9467	2.45065	0.18321
H	2.20001	2.83771	1.39478
H	2.53442	3.06889	-0.34445
C	2.10613	-2.41595	-0.37577
H	1.08346	-2.37204	-0.75474
H	2.76199	-2.83233	-1.14787
H	2.13732	-3.06042	0.50983
C	-1.07965	-2.31367	1.06763
H	-0.86738	-2.49856	0.03532
H	-0.29472	-1.72396	1.4931
H	-1.1492	-3.245	1.58982

A2

E= -786.0759253
ZPE= 0.309256
$\mathbf{H}_{corr}$= 0.327544
$\mathbf{G}_{corr}$= 0.262062
$\mathbf{E}_{tot}$= -785.813863
$\mathbf{H}_{tot}$= -785.748382
$\mathbf{G}_{tot}$= -785.76667

C	-3.24027	0.41031	0.66801
C	-2.97752	-0.91917	-0.11733
C	-1.99574	-0.5023	-1.20339
C	-1.84487	0.89125	-1.24821
C	-2.70282	1.57592	-0.18915
H	-3.84627	-1.43419	-0.55028
H	-1.82618	-1.15413	-2.06143
H	-1.54209	1.44035	-2.14155
H	-3.52929	2.12255	-0.67053
H	-2.15355	2.31436	0.41329
H	-4.28076	0.55857	0.97446
C	-2.36088	-0.14104	1.82961
H	-1.34947	0.28166	1.81403
H	-2.76862	-0.04379	2.84205
C	-2.41477	-1.5559	1.18945
H	-3.14802	-2.20736	1.67887
Ni	-0.16502	0.06187	-0.61398
C	1.669	0.0213	-0.09396

TS-A2

E= -786.0174929
ZPE= 0.30817
$\mathbf{H}_{corr}$= 0.325835
$\mathbf{G}_{corr}$= 0.26315
$\mathbf{E}_{tot}$= -785.752997
$\mathbf{H}_{tot}$= -785.734903
$\mathbf{G}_{tot}$= -785.798966

one imaginary frequency = -304.70 cm^{-1}

C	-3.02989	0.25482	0.56867
C	-2.50643	-0.91228	-0.29599
C	-1.99172	-0.36285	-1.53824
C	-1.6974	1.00019	-1.3591
C	-2.44574	1.53037	-0.13023
H	-3.07969	-1.83614	-0.33914
H	-1.81559	-0.9327	-2.44723
H	-1.42188	1.66354	-2.17412
H	-3.24991	2.2202	-0.43074
H	-1.80207	2.09553	0.55909
H	-4.12538	0.31451	0.61003
C	-2.36559	-0.18627	1.89105
H	-1.77463	0.60834	2.36259
H	-3.08827	-0.53866	2.63909

C	-1.49616	-1.32559	1.31587
H	-1.89758	-2.32532	1.49653
Ni	-0.3574	-0.31228	-0.42674
C	1.46128	0.02044	-0.03349
C	3.7173	-0.31181	0.20904
C	3.48713	1.01581	0.36083
H	4.63635	-0.87738	0.23819
H	4.16516	1.8307	0.56466
N	2.11986	1.20319	0.20737
N	2.48178	-0.90443	-0.0166
C	1.4477	2.48731	0.30326
H	0.5156	2.4159	-0.25942
H	1.22306	2.74354	1.34539
H	2.08083	3.26898	-0.1279
C	2.28654	-2.31704	-0.29161
H	1.23918	-2.55927	-0.09703
H	2.51522	-2.55399	-1.33725
H	2.92902	-2.91753	0.36045
C	-0.02982	-1.32693	1.78644
H	0.56715	-1.88022	1.09189
H	0.32805	-0.32005	1.8414
H	0.03417	-1.78145	2.75299

B2

E= -786.0632974
ZPE= 0.308562
$\mathbf{H}_{corr}$= 0.326621
$\mathbf{G}_{corr}$= 0.263809
$\mathbf{E}_{tot}$= -785.754736
$\mathbf{H}_{tot}$= -785.736677
$\mathbf{G}_{tot}$= -785.799489

C	-2.82003	0.08823	0.62232
C	-2.46943	-0.81242	-0.56688
C	-2.05823	-0.04398	-1.68356
C	-1.66105	1.22282	-1.24534
C	-2.30014	1.49547	0.12262
H	-2.82055	-1.83655	-0.63766
H	-1.89295	-0.43334	-2.68467
H	-1.31778	2.01512	-1.90391
H	-3.13073	2.21076	0.01885
H	-1.60156	1.93955	0.84477
H	-3.90515	0.14681	0.8076
C	-2.0818	-0.48405	1.86449
H	-1.78349	0.33781	2.53059
H	-2.77424	-1.10837	2.453
C	-0.83779	-1.30226	1.39767
H	-1.08611	-2.36691	1.30641
Ni	-0.49589	-0.38382	-0.32733
C	1.34606	0.05923	-0.11974
C	3.59078	-0.29988	0.08676
C	3.37215	1.02004	0.30807
H	4.50443	-0.87441	0.08114
H	4.0549	1.82052	0.54851
N	2.00489	1.22359	0.17019
N	2.35165	-0.86976	-0.16549
C	1.34636	2.50421	0.36951
H	0.46556	2.5426	-0.27116
H	1.03724	2.63097	1.41289
H	2.03287	3.31109	0.09847
C	2.13696	-2.27542	-0.47734
H	1.09674	-2.51176	-0.24257
H	2.32574	-2.47515	-1.53799
H	2.80608	-2.89259	0.12961
C	0.33143	-1.18415	2.39296
H	0.01622	-1.52803	3.35592
H	1.15164	-1.78076	2.05207
H	0.63879	-0.1616	2.46241

TS-B2

E= -786.0337952
ZPE= 0.307296
$\mathbf{H}_{corr}$= 0.325188
$\mathbf{G}_{corr}$= 0.261335
$\mathbf{E}_{tot}$= -785.726499
$\mathbf{H}_{tot}$= -785.708607
$\mathbf{G}_{tot}$= -785.77246

one imaginary frequency = -217.39 cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033
C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-3.44835	-1.46956	1.41438
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654

H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	-0.71277	-0.54087	2.13269
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549
H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995
H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
C	0.52181	1.21673	2.17198
H	1.41579	0.6328	2.24085
H	0.70511	2.07947	1.56619
H	0.2214	1.52586	3.15131

C2

E= -786.0612793
ZPE= 0.308283
$\mathbf{H}_{corr}$= 0.326376
$\mathbf{G}_{corr}$= 0.262314
$\mathbf{E}_{tot}$= -785.752997
$\mathbf{H}_{tot}$= -785.734903
$\mathbf{G}_{tot}$= -785.798966

C	3.38544	-0.70088	0.35188
C	3.62143	0.7761	0.60668
C	2.8094	1.49501	-0.19498
C	2.00875	0.60011	-1.06473
C	2.86564	-0.66987	-1.10316
H	4.24159	1.16354	1.41048
H	2.69264	2.57668	-0.16316
H	1.71139	1.01621	-2.05005
H	3.7166	-0.55709	-1.79483
H	2.32101	-1.58255	-1.37841
H	4.27961	-1.32544	0.47557
C	2.25143	-1.25223	1.27174
H	2.0473	-2.29128	0.97184
H	2.64141	-1.30459	2.30078
C	0.95569	-0.44483	1.25667
H	1.06764	0.4939	1.81619
Ni	0.23753	0.2524	-0.40606
C	-1.72097	0.05051	-0.13083
C	-3.91749	0.47413	0.31565
C	-3.79496	-0.86404	0.11842
H	-4.78102	1.07723	0.55222
H	-4.53153	-1.65263	0.15002
N	-2.45627	-1.10083	-0.15372
N	-2.64864	1.01165	0.15956
C	-1.88896	-2.41513	-0.42771
H	-0.81029	-2.29206	-0.53394
H	-2.09974	-3.09986	0.39982
H	-2.30491	-2.82723	-1.35301
C	-2.32977	2.4262	0.3014
H	-1.24424	2.52791	0.25218
H	-2.78985	3.01008	-0.5028
H	-2.68497	2.79932	1.26711
C	-0.19205	-1.25913	1.88215
H	-1.032	-0.61864	2.05287
H	-0.47427	-2.04753	1.21604
H	0.13267	-1.67702	2.81211

TS-C2

E= -786.027357
ZPE= 0.307598
$\mathbf{H}_{corr}$= 0.325391
$\mathbf{G}_{corr}$= 0.261615
$\mathbf{E}_{tot}$= -785.719759
$\mathbf{H}_{tot}$= -785.701966
$\mathbf{G}_{tot}$= -785.765742

one imaginary frequency = -320.84 cm^{-1}

C	3.84554	-0.57717	0.11783
C	4.01579	0.87636	-0.27487

C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	4.89943	1.47283	-0.06965
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	1.59154	1.06181	1.53926
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335
H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
C	0.51671	-0.7837	1.86101
H	-0.33125	-0.15367	2.03106
H	0.23435	-1.59848	1.22752
H	0.87098	-1.16497	2.7959

D2

E= -786.0535307
ZPE= 0.310689
$\mathbf{H}_{corr}$= 0.327641
$\mathbf{G}_{corr}$= 0.265164
$\mathbf{E}_{tot}$= -785.742841
$\mathbf{H}_{tot}$= -785.72589
$\mathbf{G}_{tot}$= -785.788367

C	-4.04126	0.70777	0.06248
C	-4.37008	-0.64916	-0.54484
C	-3.214	-1.2157	-0.92067
C	-2.09712	-0.24046	-0.57892
C	-2.82129	1.10829	-0.79872
H	-5.35697	-1.10172	-0.55373
H	-3.05803	-2.22327	-1.29334
H	-1.16241	-0.39221	-1.17281
H	-3.07472	1.27983	-1.84947
H	-2.26655	1.96762	-0.40397
H	-4.86531	1.42256	0.12885
C	-3.32556	0.42555	1.42801
H	-3.12639	1.3668	1.95284
H	-3.92612	-0.20529	2.08973
C	-1.99463	-0.273	0.99694
H	-1.91696	-1.29456	1.37644
Ni	0.19964	-0.10871	0.08665
C	2.00683	-0.00421	0.01204
C	4.23369	-0.55286	-0.05884
C	4.15169	0.79847	-0.12843
H	5.09203	-1.20775	-0.05591
H	4.92449	1.54863	-0.20392
N	2.80218	1.12095	-0.07971
N	2.93219	-1.02919	0.02537
C	2.27791	2.47183	-0.15897
H	1.21875	2.42597	0.10241
H	2.80346	3.12644	0.54529
H	2.38099	2.8787	-1.17235
C	2.57753	-2.43279	0.12484
H	1.48723	-2.49007	0.13995
H	2.96095	-2.99225	-0.7365
H	2.97785	-2.87367	1.04557
C	-0.79938	0.51906	1.55873
H	-0.72908	0.35784	2.61418
H	0.10176	0.18761	1.08651
H	-0.94033	1.56205	1.36585

1-2

E= -311.9813039
ZPE= 0.180564
$\mathbf{H}_{corr}$= 0.18865
$\mathbf{G}_{corr}$= 0.149373
$\mathbf{E}_{tot}$= -311.80074
$\mathbf{H}_{tot}$= -311.792654
$\mathbf{G}_{tot}$= -311.831931

C	-0.18783	-0.80949	0.57258
C	-0.3781	0.7581	0.63845
C	0.85414	1.28263	-0.07204
C	1.72819	0.29949	-0.3872
C	1.25617	-1.07851	0.06872
H	-0.52543	1.22079	1.62262
H	0.99869	2.33779	-0.29411
H	2.67575	0.45146	-0.89981
H	1.90982	-1.47509	0.86103
H	1.27134	-1.81468	-0.74939
H	-0.42464	-1.34962	1.49504
C	-1.33823	-0.87747	-0.49571
H	-0.96272	-1.0677	-1.50788
H	-2.14394	-1.5887	-0.28452
C	-1.68006	0.63201	-0.23626
C	-1.74491	1.5368	-1.48074
H	-2.71695	1.46666	-1.92245
H	-1.55524	2.55037	-1.19508
H	-1.00758	1.22202	-2.18938
H	-2.57601	0.76615	0.33312

2-2

E= -311.989139
ZPE= 0.181858
$\mathbf{H}_{corr}$= 0.189431
$\mathbf{G}_{corr}$= 0.151567
$\mathbf{E}_{tot}$= -311.807281
$\mathbf{H}_{tot}$= -311.799709
$\mathbf{G}_{tot}$= -311.837572

C	-0.08784	-1.13781	0.32395
C	-1.28896	-0.67849	-0.51196
C	-1.28889	0.67866	-0.5119
C	-0.0877	1.13776	0.32407
C	-0.03905	-0.00011	1.39044
H	-1.94331	-1.3387	-1.07286
H	-1.94296	1.33932	-1.07258
H	-0.11891	2.16699	0.68974
H	-0.90918	-0.00011	2.05524
H	0.88406	-0.00019	1.98484
H	-0.11913	-2.16709	0.68946
C	1.20038	-0.78595	-0.52016
H	2.09804	-1.18453	-0.03039
H	1.15122	-1.20753	-1.52983
C	1.20049	0.78591	-0.52006
H	1.1514	1.20766	-1.52967
C	2.46011	1.34493	0.16729
H	3.28531	1.30411	-0.51262
H	2.28714	2.36014	0.45771
H	2.68307	0.75897	1.03438

A3

E= -786.0765513
ZPE 0.309222
$\mathbf{H}_{corr}$ 0.327683
$\mathbf{G}_{corr}$= 0.260518
$\mathbf{E}_{tot}$= -785.76733
$\mathbf{H}_{tot}$= -785.748869
$\mathbf{G}_{tot}$= -785.816034

C	-3.24027	0.41031	0.66801
C	-2.97752	-0.91917	-0.11733
C	-1.99574	-0.5023	-1.20339
C	-1.84487	0.89125	-1.24821
C	-2.70282	1.57592	-0.18915
H	-3.84627	-1.43419	-0.55028
H	-1.82618	-1.15413	-2.06143
H	-1.54209	1.44035	-2.14155
H	-3.52929	2.12255	-0.67053
H	-2.15355	2.31436	0.41329
H	-4.28076	0.55857	0.97446
C	-2.36088	-0.14104	1.82961
H	-1.34947	0.28166	1.81403
H	-2.76862	-0.04379	2.84205
C	-2.41477	-1.5559	1.18945
H	-1.4652	-2.09484	1.10281
Ni	-0.16502	0.06187	-0.61398
C	1.669	0.0213	-0.09396
C	3.78847	-0.69974	0.36787
C	3.76353	0.63974	0.5806
H	4.58918	-1.41632	0.47139
H	4.5398	1.31835	0.90032
N	2.47137	1.06194	0.29911
N	2.51242	-1.05943	-0.04341
C	2.01817	2.44096	0.39016
H	0.9467	2.45065	0.18321

H	2.20001	2.83771	1.39478
H	2.53442	3.06889	-0.34445
C	2.10613	-2.41595	-0.37577
H	1.08346	-2.37204	-0.75474
H	2.76199	-2.83233	-1.14787
H	2.13732	-3.06042	0.50983
C	-3.4449	-2.47113	1.87703
H	-3.57961	-3.35793	1.29364
H	-3.09227	-2.73573	2.85198
H	-4.37858	-1.95564	1.96319

TS-A3

E= -786.0270214
ZPE=0.307415
$\mathbf{H}_{corr}$ = 0.325416
$\mathbf{G}_{corr}$= 0.261454
$\mathbf{E}_{tot}$= -785.719606
$\mathbf{H}_{tot}$= -785.701606
$\mathbf{G}_{tot}$= -785.765568

one imaginary frequency = -385.30 cm^{-1}

C	-3.02989	0.25482	0.56867
C	-2.50643	-0.91228	-0.29599
C	-1.99172	-0.36285	-1.53824
C	-1.6974	1.00019	-1.3591
C	-2.44574	1.53037	-0.13023
H	-3.07969	-1.83614	-0.33914
H	-1.81559	-0.9327	-2.44723
H	-1.42188	1.66354	-2.17412
H	-3.24991	2.2202	-0.43074
H	-1.80207	2.09553	0.55909
H	-4.12538	0.31451	0.61003
C	-2.36559	-0.18627	1.89105
H	-1.77463	0.60834	2.36259
H	-3.08827	-0.53866	2.63909
C	-1.49616	-1.32559	1.31587
H	-0.45581	-1.32654	1.64974
Ni	-0.3574	-0.31228	-0.42674
C	1.46128	0.02044	-0.03349
C	3.7173	-0.31181	0.20904
C	3.48713	1.01581	0.36083
H	4.63635	-0.87738	0.23819
H	4.16516	1.8307	0.56466
N	2.11986	1.20319	0.20737
N	2.48178	-0.90443	-0.0166
C	1.4477	2.48731	0.30326
H	0.5156	2.4159	-0.25942
H	1.22306	2.74354	1.34539
H	2.08083	3.26898	-0.1279
C	2.28654	-2.31704	-0.29161
H	1.23918	-2.55927	-0.09703
H	2.51522	-2.55399	-1.33725
H	2.92902	-2.91753	0.36045
C	-2.06208	-2.73501	1.57057
H	-1.62739	-3.1383	2.46124
H	-3.1242	-2.67728	1.68659
H	-1.82785	-3.36871	0.74083

B3

E= -786.0622699
ZPE= 0.308514
$\mathbf{H}_{corr}$= 0.32663
$\mathbf{G}_{corr}$= 0.26352
$\mathbf{E}_{tot}$= -785.753756
$\mathbf{H}_{tot}$= -785.73564
$\mathbf{G}_{tot}$= -785.79875

C	-2.82003	0.08823	0.62232
C	-2.46943	-0.81242	-0.56688
C	-2.05823	-0.04398	-1.68356
C	-1.66105	1.22282	-1.24534
C	-2.30014	1.49547	0.12262
H	-2.82055	-1.83655	-0.63766
H	-1.89295	-0.43334	-2.68467
H	-1.31778	2.01512	-1.90391
H	-3.13073	2.21076	0.01885
H	-1.60156	1.93955	0.84477
H	-3.90515	0.14681	0.8076
C	-2.0818	-0.48405	1.86449
H	-1.78349	0.33781	2.53059
H	-2.77424	-1.10837	2.453
C	-0.83779	-1.30226	1.39767
H	-0.00477	-1.21811	2.10677
Ni	-0.49589	-0.38382	-0.32733
C	1.34606	0.05923	-0.11974
C	3.59078	-0.29988	0.08676
C	3.37215	1.02004	0.30807

H	4.50443	-0.87441	0.08114
H	4.0549	1.82052	0.54851
N	2.00489	1.22359	0.17019
N	2.35165	-0.86976	-0.16549
C	1.34636	2.50421	0.36951
H	0.46556	2.5426	-0.27116
H	1.03724	2.63097	1.41289
H	2.03287	3.31109	0.09847
C	2.13696	-2.27542	-0.47734
H	1.09674	-2.51176	-0.24257
H	2.32574	-2.47515	-1.53799
H	2.80608	-2.89259	0.12961
C	-1.18638	-2.7968	1.26956
H	-0.56367	-3.36598	1.92772
H	-2.213	-2.94727	1.53091
H	-1.02467	-3.11558	0.26103

TS-B3

E= -786.0326391
ZPE= 0.307531
$\mathbf{H}_{corr}$ = 0.325424
$\mathbf{G}_{corr}$= 0.261988
$\mathbf{E}_{tot}$= -785.725108
$\mathbf{H}_{tot}$= -785.707215
$\mathbf{G}_{tot}$= -785.770651

one imaginary frequency = -228.32 cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033
C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-3.44835	-1.46956	1.41438
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654
H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	0.19853	0.97206	1.98788
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549
H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995
H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
C	-0.75996	-0.91012	2.37475
H	0.10637	-1.04816	2.98738
H	-1.62603	-0.82061	2.99669
H	-0.87396	-1.75138	1.72346

C3

E= -786.0599972
ZPE= 0.308568
$\mathbf{H}_{corr}$ = 0.326583
$\mathbf{G}_{corr}$= 0.263234
$\mathbf{E}_{tot}$= -785.75143
$\mathbf{H}_{tot}$= -785.733415
$\mathbf{G}_{tot}$= -785.796763

C	3.38544	-0.70088	0.35188
C	3.62143	0.7761	0.60668
C	2.8094	1.49501	-0.19498
C	2.00875	0.60011	-1.06473
C	2.86564	-0.66987	-1.10316
H	4.24159	1.16354	1.41048
H	2.69264	2.57668	-0.16316
H	1.71139	1.01621	-2.05005
H	3.7166	-0.55709	-1.79483
H	2.32101	-1.58255	-1.37841
H	4.27961	-1.32544	0.47557
C	2.25143	-1.25223	1.27174
H	2.0473	-2.29128	0.97184
H	2.64141	-1.30459	2.30078

C	0.95569	-0.44483	1.25667
H	0.13706	-1.02564	1.70279
Ni	0.23753	0.2524	-0.40606
C	-1.72097	0.05051	-0.13083
C	-3.91749	0.47413	0.31565
C	-3.79496	-0.86404	0.11842
H	-4.78102	1.07723	0.55222
H	-4.53153	-1.65263	0.15002
N	-2.45627	-1.10083	-0.15372
N	-2.64864	1.01165	0.15956
C	-1.88896	-2.41513	-0.42771
H	-0.81029	-2.29206	-0.53394
H	-2.09974	-3.09986	0.39982
H	-2.30491	-2.82723	-1.35301
C	-2.32977	2.4262	0.3014
H	-1.24424	2.52791	0.25218
H	-2.78985	3.01008	-0.5028
H	-2.68497	2.79932	1.26711
C	1.11264	0.87113	2.04103
H	0.2635	1.01077	2.67693
H	2.00072	0.8278	2.63628
H	1.18273	1.68914	1.35485

TS-C3

E= -786.0271478
ZPE= 0.307279
$\mathbf{H}_{corr}$ = 0.325149
$\mathbf{G}_{corr}$= 0.260825
$\mathbf{E}_{tot}$= -785.719868
$\mathbf{H}_{tot}$= -785.701999
$\mathbf{G}_{tot}$= -785.766323

one imaginary frequency = -336.16 cm^{-1}

C	3.84554	-0.57717	0.11783
C	4.01579	0.87636	-0.27487
C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	4.89943	1.47283	-0.06965
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	0.83076	-0.55465	1.67022
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335
H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
C	1.57425	1.48514	1.68578
H	0.78183	1.584	2.39795
H	2.50426	1.74041	2.14928
H	1.39541	2.14142	0.85981

D3

E= -786.0465122
ZPE= 0.309867
$\mathbf{H}_{corr}$ = 0.327451
$\mathbf{G}_{corr}$= 0.263257
$\mathbf{E}_{tot}$= -785.736645
$\mathbf{H}_{tot}$= -785.719062
$\mathbf{G}_{tot}$= -785.783256

C	-4.04126	0.70777	0.06248
C	-4.37008	-0.64916	-0.54484
C	-3.214	-1.2157	-0.92067
C	-2.09712	-0.24046	-0.57892
C	-2.82129	1.10829	-0.79872
H	-5.35697	-1.10172	-0.55373
H	-3.05803	-2.22327	-1.29334

H	-1.16241	-0.39221	-1.17281
H	-3.07472	1.27983	-1.84947
H	-2.26655	1.96762	-0.40397
H	-4.86531	1.42256	0.12885
C	-3.32556	0.42555	1.42801
H	-3.12639	1.3668	1.95284
H	-3.92612	-0.20529	2.08973
C	-1.99463	-0.273	0.99694
H	-1.12497	0.3033	1.4057
Ni	0.19964	-0.10871	0.08665
C	2.00683	-0.00421	0.01204
C	4.23369	-0.55286	-0.05884
C	4.15169	0.79847	-0.12843
H	5.09203	-1.20775	-0.05591
H	4.92449	1.54863	-0.20392
N	2.80218	1.12095	-0.07971
N	2.93219	-1.02919	0.02537
C	2.27791	2.47183	-0.15897
H	1.21875	2.42597	0.10241
H	2.80346	3.12644	0.54529
H	2.38099	2.8787	-1.17235
C	2.57753	-2.43279	0.12484
H	1.48723	-2.49007	0.13995
H	2.96095	-2.99225	-0.7365
H	2.97785	-2.87367	1.04557
C	-1.88514	-1.71295	1.53187
H	-1.2919	-2.29851	0.86099
H	-1.42432	-1.70065	2.49747
H	-2.86313	-2.14018	1.60881

1-3

E= -311.9816166
ZPE= 0.18044
$\mathbf{H}_{corr}$ = 0.188617
$\mathbf{G}_{corr}$= 0.148957
$\mathbf{E}_{tot}$= -311.801177
$\mathbf{H}_{tot}$= -311.792999
$\mathbf{G}_{tot}$= -311.83266

C	-0.18783	-0.80949	0.57258
C	-0.3781	0.7581	0.63845
C	0.85414	1.28263	-0.07204
C	1.72819	0.29949	-0.3872
C	1.25617	-1.07851	0.06872
H	-0.52543	1.22079	1.62262
H	0.99869	2.33779	-0.29411
H	2.67575	0.45146	-0.89981
H	1.90982	-1.47509	0.86103
H	1.27134	-1.81468	-0.74939
H	-0.42464	-1.34962	1.49504
C	-1.33823	-0.87747	-0.49571
H	-0.96272	-1.0677	-1.50788
H	-2.14394	-1.5887	-0.28452
C	-1.68006	0.63201	-0.23626
H	-1.72619	1.27559	-1.12146
C	-2.96956	0.82508	0.58322
H	-3.06021	1.85226	0.86883
H	-3.81455	0.5439	-0.00993
H	-2.92985	0.21322	1.46012

2-3

E= -311.9891864
ZPE= 0.181866
$\mathbf{H}_{corr}$ = 0.189429
$\mathbf{G}_{corr}$= 0.151585
$\mathbf{E}_{tot}$= -311.807321
$\mathbf{H}_{tot}$= -311.799757
$\mathbf{G}_{tot}$= -311.837601

C	-0.08784	-1.13781	0.32395
C	-1.28896	-0.67849	-0.51196
C	-1.28889	0.67866	-0.5119
C	-0.0877	1.13776	0.32407
C	-0.03905	-0.00011	1.39044
H	-1.94331	-1.3387	-1.07286
H	-1.94296	1.33932	-1.07258
H	-0.11891	2.16699	0.68974
H	-0.90918	-0.00011	2.05524
H	0.88406	-0.00019	1.98484
H	-0.11913	-2.16709	0.68946
C	1.20038	-0.78595	-0.52016
H	2.09804	-1.18453	-0.03039
H	1.15122	-1.20753	-1.52983
C	1.20049	0.78591	-0.52006
C	1.13147	1.37892	-1.93963
H	0.7744	2.38629	-1.88838

H	2.10729	1.36829	-2.37844
H	0.46475	0.79422	-2.53839
H	2.07568	1.17432	-0.04248

A4

E= -951.2482555
ZPE= 0.283417
$\mathbf{H}_{corr}$ = 0.30299
$\mathbf{G}_{corr}$= 0.231974
$\mathbf{E}_{tot}$= -950.964839
$\mathbf{H}_{tot}$= -950.945265
$\mathbf{G}_{tot}$= -951.016282

C	-3.24027	0.41031	0.66801
C	-2.97752	-0.91917	-0.11733
C	-1.99574	-0.5023	-1.20339
C	-1.84487	0.89125	-1.24821
C	-2.70282	1.57592	-0.18915
H	-3.84627	-1.43419	-0.55028
H	-1.82618	-1.15413	-2.06143
H	-1.54209	1.44035	-2.14155
H	-3.52929	2.12255	-0.67053
H	-2.15355	2.31436	0.41329
H	-4.28076	0.55857	0.97446
C	-2.36088	-0.14104	1.82961
H	-1.34947	0.28166	1.81403
H	-2.76862	-0.04379	2.84205
C	-2.41477	-1.5559	1.18945
H	-1.4652	-2.09484	1.10281
Ni	-0.16502	0.06187	-0.61398
C	1.669	0.0213	-0.09396
C	3.78847	-0.69974	0.36787
C	3.76353	0.63974	0.5806
H	4.58918	-1.41632	0.47139
H	4.5398	1.31835	0.90032
N	2.47137	1.06194	0.29911
N	2.51242	-1.05943	-0.04341
C	2.01817	2.44096	0.39016
H	0.9467	2.45065	0.18321
H	2.20001	2.83771	1.39478
H	2.53442	3.06889	-0.34445
C	2.10613	-2.41595	-0.37577
H	1.08346	-2.37204	-0.75474
H	2.76199	-2.83233	-1.14787
H	2.13732	-3.06042	0.50983
N	-3.39808	-2.42953	1.84577
O	-3.97144	-3.24489	1.17879
O	-3.58769	-2.29204	3.02202

TS-A4

E= -951.219692
ZPE= 0.282013
$\mathbf{H}_{corr}$ = 0.300933
$\mathbf{G}_{corr}$= 0.234651
$\mathbf{E}_{tot}$= -950.937679
$\mathbf{H}_{tot}$= -950.918759
$\mathbf{G}_{tot}$= -950.985041

one imaginary frequency = -338.57 cm^{-1}

C	-3.02989	0.25482	0.56867
C	-2.50643	-0.91228	-0.29599
C	-1.99172	-0.36285	-1.53824
C	-1.6974	1.00019	-1.3591
C	-2.44574	1.53037	-0.13023
H	-3.07969	-1.83614	-0.33914
H	-1.81559	-0.9327	-2.44723
H	-1.42188	1.66354	-2.17412
H	-3.24991	2.2202	-0.43074
H	-1.80207	2.09553	0.55909
H	-4.12538	0.31451	0.61003
C	-2.36559	-0.18627	1.89105
H	-1.77463	0.60834	2.36259
H	-3.08827	-0.53866	2.63909
C	-1.49616	-1.32559	1.31587
H	-0.45581	-1.32654	1.64974
Ni	-0.3574	-0.31228	-0.42674
C	1.46128	0.02044	-0.03349
C	3.7173	-0.31181	0.20904
C	3.48713	1.01581	0.36083
H	4.63635	-0.87738	0.23819
H	4.16516	1.8307	0.56466
N	2.11986	1.20319	0.20737
N	2.48178	-0.90443	-0.0166
C	1.4477	2.48731	0.30326
H	0.5156	2.4159	-0.25942
H	1.22306	2.74354	1.34539
H	2.08083	3.26898	-0.1279

C	2.28654	-2.31704	-0.29161
H	1.23918	-2.55927	-0.09703
H	2.51522	-2.55399	-1.33725
H	2.92902	-2.91753	0.36045
N	-2.03635	-2.67094	1.55899
O	-2.08863	-3.43926	0.63954
O	-2.40323	-2.94653	2.66708
H	2.03287	3.31109	0.09847
C	2.13696	-2.27542	-0.47734
H	1.09674	-2.51176	-0.24257
H	2.32574	-2.47515	-1.53799
H	2.80608	-2.89259	0.12961
N	-1.17053	-2.72887	1.27538
O	-2.29238	-3.0292	0.97591
O	-0.30687	-3.53549	1.47996

B4

E= -951.2665489
ZPE= 0.283767
$\mathbf{H}_{corr}$ = 0.30256
$\mathbf{G}_{corr}$= 0.237974
$\mathbf{E}_{tot}$= -950.982782
$\mathbf{H}_{tot}$= -950.963989
$\mathbf{G}_{tot}$= -951.028575

C	-2.82003	0.08823	0.62232
C	-2.46943	-0.81242	-0.56688
C	-2.05823	-0.04398	-1.68356
C	-1.66105	1.22282	-1.24534
C	-2.30014	1.49547	0.12262
H	-2.82055	-1.83655	-0.63766
H	-1.89295	-0.43334	-2.68467
H	-1.31778	2.01512	-1.90391
H	-3.13073	2.21076	0.01885
H	-1.60156	1.93955	0.84477
H	-3.90515	0.14681	0.8076
C	-2.0818	-0.48405	1.86449
H	-1.78349	0.33781	2.53059
H	-2.77424	-1.10837	2.453
C	-0.83779	-1.30226	1.39767
H	-0.00477	-1.21811	2.10677
Ni	-0.49589	-0.38382	-0.32733
C	1.34606	0.05923	-0.11974
C	3.59078	-0.29988	0.08676
C	3.37215	1.02004	0.30807
H	4.50443	-0.87441	0.08114
H	4.0549	1.82052	0.54851
N	2.00489	1.22359	0.17019
N	2.35165	-0.86976	-0.16549
C	1.34636	2.50421	0.36951
H	0.46556	2.5426	-0.27116
H	1.03724	2.63097	1.41289

TS-B4

E= -951.219692
ZPE= 0.282013
$\mathbf{H}_{corr}$ = 0.300933
$\mathbf{G}_{corr}$= 0.234651
$\mathbf{E}_{tot}$= -950.937679
$\mathbf{H}_{tot}$= -950.918759
$\mathbf{G}_{tot}$= -950.985041

one imaginary frequency = -852.35 cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033
C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-3.44835	-1.46956	1.41438
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654
H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	0.19853	0.97206	1.98788
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549
H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995

H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
N	-0.75252	-0.85191	2.33659
O	-1.86045	-1.26625	2.53468
O	0.23416	-1.38608	2.76028
H	-0.81029	-2.29206	-0.53394
H	-2.09974	-3.09986	0.39982
H	-2.30491	-2.82723	-1.35301
C	-2.32977	2.4262	0.3014
H	-1.24424	2.52791	0.25218
H	-2.78985	3.01008	-0.5028
H	-2.68497	2.79932	1.26711
N	1.1055	0.81131	2.00537
O	1.2166	1.83349	1.38793
O	1.11065	0.76381	3.20376

C4

E= -951.2808957
ZPE= 0.283931
$\mathbf{H}_{corr}$ = 0.302679
$\mathbf{G}_{corr}$= 0.237902
$\mathbf{E}_{tot}$= -950.996964
$\mathbf{H}_{tot}$= -950.978216
$\mathbf{G}_{tot}$= -951.042994

C	3.38544	-0.70088	0.35188
C	3.62143	0.7761	0.60668
C	2.8094	1.49501	-0.19498
C	2.00875	0.60011	-1.06473
C	2.86564	-0.66987	-1.10316
H	4.24159	1.16354	1.41048
H	2.69264	2.57668	-0.16316
H	1.71139	1.01621	-2.05005
H	3.7166	-0.55709	-1.79483
H	2.32101	-1.58255	-1.37841
H	4.27961	-1.32544	0.47557
C	2.25143	-1.25223	1.27174
H	2.0473	-2.29128	0.97184
H	2.64141	-1.30459	2.30078
C	0.95569	-0.44483	1.25667
H	0.13706	-1.02564	1.70279
Ni	0.23753	0.2524	-0.40606
C	-1.72097	0.05051	-0.13083
C	-3.91749	0.47413	0.31565
C	-3.79496	-0.86404	0.11842
H	-4.78102	1.07723	0.55222
H	-4.53153	-1.65263	0.15002
N	-2.45627	-1.10083	-0.15372
N	-2.64864	1.01165	0.15956
C	-1.88896	-2.41513	-0.42771

TS-C4

E= -951.2219272
ZPE= 0.282519
$\mathbf{H}_{corr}$= 0.301218
$\mathbf{G}_{corr}$= 0.23486
$\mathbf{E}_{tot}$= -950.939409
$\mathbf{H}_{tot}$= -950.920709
$\mathbf{G}_{tot}$= -950.987067

one imaginary frequency = -318.29 cm^{-1}

C	3.84554	-0.57717	0.11783
C	4.01579	0.87636	-0.27487
C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	4.89943	1.47283	-0.06965
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	0.83076	-0.55465	1.67022
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335

H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
N	1.57695	1.41904	1.6629
O	1.84209	2.3001	0.89357
O	1.26782	1.61506	2.80501
H	5.09203	-1.20775	-0.05591
H	4.92449	1.54863	-0.20392
N	2.80218	1.12095	-0.07971
N	2.93219	-1.02919	0.02537
C	2.27791	2.47183	-0.15897
H	1.21875	2.42597	0.10241
H	2.80346	3.12644	0.54529
H	2.38099	2.8787	-1.17235
C	2.57753	-2.43279	0.12484
H	1.48723	-2.49007	0.13995
H	2.96095	-2.99225	-0.7365
H	2.97785	-2.87367	1.04557
N	-1.89012	-1.6475	1.50755
O	-2.66831	-2.00463	2.34737
O	-1.03083	-2.35688	1.06393

D4

E= -951.2543002
ZPE= 0.285492
$\mathbf{H}_{corr}$ = 0.304525
$\mathbf{G}_{corr}$= 0.235024
$\mathbf{E}_{tot}$= -950.968808
$\mathbf{H}_{tot}$= -950.949775
$\mathbf{G}_{tot}$= -951.019277

C	-4.04126	0.70777	0.06248
C	-4.37008	-0.64916	-0.54484
C	-3.214	-1.2157	-0.92067
C	-2.09712	-0.24046	-0.57892
C	-2.82129	1.10829	-0.79872
H	-5.35697	-1.10172	-0.55373
H	-3.05803	-2.22327	-1.29334
H	-1.16241	-0.39221	-1.17281
H	-3.07472	1.27983	-1.84947
H	-2.26655	1.96762	-0.40397
H	-4.86531	1.42256	0.12885
C	-3.32556	0.42555	1.42801
H	-3.12639	1.3668	1.95284
H	-3.92612	-0.20529	2.08973
C	-1.99463	-0.273	0.99694
H	-1.12497	0.3033	1.4057
Ni	0.19964	-0.10871	0.08665
C	2.00683	-0.00421	0.01204
C	4.23369	-0.55286	-0.05884
C	4.15169	0.79847	-0.12843

1-4

E= -477.1478378
ZPE= 0.15436
$\mathbf{H}_{corr}$ = 0.163678
$\mathbf{G}_{corr}$= 0.119724
$\mathbf{E}_{tot}$= -476.993478
$\mathbf{H}_{tot}$= -476.98416
$\mathbf{G}_{tot}$= -477.028114

C	0.6728	-1.01414	0.42575
C	-0.10056	0.25601	0.95986
C	0.59764	1.39741	0.24557
C	1.69396	0.99106	-0.43524
C	1.94224	-0.5095	-0.31078
H	-0.15212	0.41873	2.04465
H	0.25145	2.42717	0.30139
H	2.35006	1.64668	-1.004
H	2.86434	-0.70854	0.2572
H	2.06497	-0.9939	-1.29146
H	0.88953	-1.77996	1.17752
C	-0.57401	-1.36027	-0.4633
H	-0.42087	-1.08283	-1.51389
H	-0.9306	-2.3955	-0.424
C	-1.43208	-0.29979	0.31461
H	-2.06041	0.3579	-0.24889
N	-2.22991	-0.96364	1.35561
O	-2.44952	-0.36746	2.37284
O	-2.62936	-2.07493	1.14611

2-4

E= -477.1552967
ZPE= 0.155827
$\mathbf{H}_{corr}$ = 0.164512
$\mathbf{G}_{corr}$= 0.122578
$\mathbf{E}_{tot}$= -476.99947
$\mathbf{H}_{tot}$= -476.990785
$\mathbf{G}_{tot}$= -477.032719

C	0.97671	1.01721	0.31727
C	1.86901	0.0747	-0.50162
C	1.27982	-1.14759	-0.49546
C	-0.01318	-1.02946	0.32144
C	0.43144	0.0205	1.38703
H	2.75354	0.37957	-1.05232
H	1.58848	-2.03236	-1.04354
H	-0.44089	-1.96706	0.68687
H	1.21222	-0.35774	2.05499
H	-0.39543	0.4288	1.98097
H	1.44945	1.93326	0.68057
C	-0.33298	1.2531	-0.52936
H	-0.98141	1.98187	-0.02459
H	-0.11107	1.6366	-1.53134
C	-1.01199	-0.16793	-0.55978
H	-2.01525	-0.17169	-0.18781
N	-1.02529	-0.69745	-1.93103
O	-0.80649	0.05818	-2.83633
O	-1.25442	-1.86395	-2.08972

A5

E= -846.0206246
ZPE= 0.273343
$\mathbf{H}_{corr}$ = 0.291138
$\mathbf{G}_{corr}$= 0.224982
$\mathbf{E}_{tot}$= -845.747282
$\mathbf{H}_{tot}$= -845.729486
$\mathbf{G}_{tot}$= -845.7956426

C	-3.24027	0.41031	0.66801
C	-2.97752	-0.91917	-0.11733
C	-1.99574	-0.5023	-1.20339
C	-1.84487	0.89125	-1.24821
C	-2.70282	1.57592	-0.18915
H	-3.84627	-1.43419	-0.55028
H	-1.82618	-1.15413	-2.06143
H	-1.54209	1.44035	-2.14155
H	-3.52929	2.12255	-0.67053
H	-2.15355	2.31436	0.41329
H	-4.28076	0.55857	0.97446
C	-2.36088	-0.14104	1.82961
H	-1.34947	0.28166	1.81403
H	-2.76862	-0.04379	2.84205
C	-2.41477	-1.5559	1.18945
H	-1.4652	-2.09484	1.10281
Ni	-0.16502	0.06187	-0.61398
C	1.669	0.0213	-0.09396
C	3.78847	-0.69974	0.36787
C	3.76353	0.63974	0.5806
H	4.58918	-1.41632	0.47139
H	4.5398	1.31835	0.90032
N	2.47137	1.06194	0.29911
N	2.51242	-1.05943	-0.04341
C	2.01817	2.44096	0.39016
H	0.9467	2.45065	0.18321
H	2.20001	2.83771	1.39478
H	2.53442	3.06889	-0.34445
C	2.10613	-2.41595	-0.37577
H	1.08346	-2.37204	-0.75474
H	2.76199	-2.83233	-1.14787
H	2.13732	-3.06042	0.50983
F	-3.31781	-2.35821	1.7922

TS-A5

E= -845.9735915
ZPE= 0.271644
$\mathbf{H}_{corr}$= 0.288836
$\mathbf{G}_{corr}$= 0.22672
$\mathbf{E}_{tot}$= -845.701948
$\mathbf{H}_{tot}$= -845.684755
$\mathbf{G}_{tot}$= -845.746871

one imaginary frequency = -428.06 cm^{-1}

C	-3.02989	0.25482	0.56867
C	-2.50643	-0.91228	-0.29599
C	-1.99172	-0.36285	-1.53824
C	-1.6974	1.00019	-1.3591

C	-2.44574	1.53037	-0.13023
H	-3.07969	-1.83614	-0.33914
H	-1.81559	-0.9327	-2.44723
H	-1.42188	1.66354	-2.17412
H	-3.24991	2.2202	-0.43074
H	-1.80207	2.09553	0.55909
H	-4.12538	0.31451	0.61003
C	-2.36559	-0.18627	1.89105
H	-1.77463	0.60834	2.36259
H	-3.08827	-0.53866	2.63909
C	-1.49616	-1.32559	1.31587
H	-0.45581	-1.32654	1.64974
Ni	-0.3574	-0.31228	-0.42674
C	1.46128	0.02044	-0.03349
C	3.7173	-0.31181	0.20904
C	3.48713	1.01581	0.36083
H	4.63635	-0.87738	0.23819
H	4.16516	1.8307	0.56466
N	2.11986	1.20319	0.20737
N	2.48178	-0.90443	-0.0166
C	1.4477	2.48731	0.30326
H	0.5156	2.4159	-0.25942
H	1.22306	2.74354	1.34539
H	2.08083	3.26898	-0.1279
C	2.28654	-2.31704	-0.29161
H	1.23918	-2.55927	-0.09703
H	2.51522	-2.55399	-1.33725
H	2.92902	-2.91753	0.36045
F	-1.99226	-2.56112	1.53914
H	-1.50881	-0.70549	2.85745
H	-0.56215	-2.79771	1.52019
H	-2.54886	-3.01552	-0.23576
H	-1.21628	-2.27319	-1.12346
H	-3.79896	-1.03539	-0.49478
C	-2.29879	0.13618	-1.58542
H	-2.057	-0.45935	-2.47784
H	-3.14083	0.78854	-1.86173
C	-1.0472	1.00376	-1.17338
H	-0.26726	0.98401	-1.94412
Ni	-0.39156	-0.08065	0.39237
C	1.4878	-0.164	0.08145
C	3.66248	0.60604	0.02597
C	3.66129	-0.64807	-0.52735
H	4.47254	1.29838	0.18852
H	4.4678	-1.2337	-0.93777
N	2.33297	-1.10621	-0.48174
N	2.33662	0.89019	0.38597
C	1.88884	-2.40102	-1.00533
H	1.02832	-2.73958	-0.42698
H	1.60112	-2.32082	-2.06073
H	2.69636	-3.13448	-0.91103
C	1.90004	2.13197	1.04216
H	0.8329	2.27466	0.86041
H	2.07828	2.08269	2.1231
H	2.44463	2.98464	0.62379
F	-1.30354	2.23809	-0.85601

B5

E= -846.0147049
ZPE= 0.272824
$\mathbf{H}_{corr}$ = 0.290218
$\mathbf{G}_{corr}$= 0.228658
$\mathbf{E}_{tot}$= -845.741881
$\mathbf{H}_{tot}$= -845.724487
$\mathbf{G}_{tot}$= -845.7860469

C	-2.72714	-0.794	-0.41021
C	-2.3917	-0.06147	0.90249
C	-1.70981	-0.92364	1.81338
C	-1.13568	-1.9887	1.07713
C	-1.88927	-2.13426	-0.26532
H	-2.89124	0.85662	1.19321

TS-B5

E= -845.9814768
ZPE= 0.272022
$\mathbf{H}_{corr}$= 0.289103
$\mathbf{G}_{corr}$= 0.227445
$\mathbf{E}_{tot}$= -845.709455
$\mathbf{H}_{tot}$= -845.692374
$\mathbf{G}_{tot}$= -845.7540318

one imaginary frequency = -266.58 cm^{-1}

C	3.07976	-0.43655	0.53633
C	3.08925	0.85159	-0.29458
C	2.42537	0.64621	-1.48006
C	1.91004	-0.74	-1.62125

C	2.75098	-1.52019	-0.55249
H	3.47551	1.79947	0.06674
H	2.25049	1.42355	-2.22261
H	1.88222	-1.17212	-2.62247
H	3.69546	-1.87447	-1.00173
H	2.24462	-2.3971	-0.12329
H	4.05588	-0.64112	1.00069
C	2.04228	-0.38145	1.70579
H	1.91437	-1.39781	2.10648
H	2.47014	0.22712	2.51972
C	0.61594	0.19176	1.3965
H	-0.12733	-0.28081	2.04932
Ni	0.29836	-0.27412	-0.4627
C	-1.54281	-0.20845	-0.20759
C	-3.72282	0.49697	-0.31407
C	-3.72955	-0.77098	0.20948
H	-4.53749	1.16973	-0.52697
H	-4.55083	-1.39409	0.52392
N	-2.39021	-1.18942	0.27354
N	-2.3827	0.8297	-0.56259
C	-1.94208	-2.50204	0.75269
H	-0.88908	-2.62302	0.48775
H	-2.05357	-2.58023	1.84067
H	-2.522	-3.29819	0.27288
C	-1.91805	2.12141	-1.09594
H	-0.98876	1.96164	-1.64882
H	-2.67452	2.52952	-1.77379
H	-1.72124	2.82776	-0.28377
F	0.46717	1.60982	1.50541

C5

E= -846.0128617
ZPE= 0.272824
$\mathbf{H}_{corr}$ 0.290218
$\mathbf{G}_{corr}$= 0.227783
$\mathbf{E}_{tot}$= -845.740038
$\mathbf{H}_{tot}$= -845.722643
$\mathbf{G}_{tot}$= -845.785078

C	3.44967	-0.54422	0.44267
C	3.57187	0.72257	-0.3932
C	2.64606	0.69078	-1.39549
C	1.87122	-0.57966	-1.33736
C	2.80896	-1.53072	-0.57437
H	4.20876	1.56289	-0.13309
H	2.44361	1.50085	-2.0919
H	1.43837	-0.95443	-2.29122
H	3.59024	-1.93675	-1.23877
H	2.29627	-2.37171	-0.08941
H	4.40529	-0.89838	0.8517
C	2.45146	-0.34544	1.64537
H	2.3907	-1.30505	2.17844
H	2.89628	0.3791	2.34261
C	1.01438	0.08396	1.27252
H	0.28038	-0.4176	1.91894
Ni	0.17214	-0.30413	-0.48596
C	-1.79322	-0.15856	-0.18476
C	-3.96708	0.60276	-0.07714
C	-3.98318	-0.72063	0.28915
H	-4.77157	1.3166	-0.14991
H	-4.80255	-1.35349	0.58981
N	-2.65702	-1.16829	0.21574
N	-2.63402	0.92787	-0.36049
C	-2.22199	-2.53405	0.53296
H	-1.13787	-2.58194	0.40486
H	-2.47403	-2.78799	1.56916
H	-2.69643	-3.25673	-0.14111
C	-2.18131	2.25644	-0.81021
H	-1.20276	2.47427	-0.37858
H	-2.12144	2.29109	-1.90407
H	-2.88976	3.01575	-0.46479
F	0.77532	1.48312	1.31232

TS-C5

E= -845.9721171
ZPE= 0.271231
$\mathbf{H}_{corr}$= 0.288378
$\mathbf{G}_{corr}$= 0.225308
$\mathbf{E}_{tot}$= -845.700887
$\mathbf{H}_{tot}$= -845.683739
$\mathbf{G}_{tot}$= -845.746809

one imaginary frequency = -389.06cm^{-1}

C	3.80121	-0.81575	0.27688
C	3.9715	0.17774	-0.86835
C	2.75797	0.34314	-1.45909
C	1.77226	-0.5799	-0.79083

C	2.67661	-1.72515	-0.28029
H	4.87925	0.73539	-1.07323
H	2.49193	1.06199	-2.2259
H	0.90818	-0.89927	-1.46243
H	3.02593	-2.34868	-1.1123
H	2.20316	-2.36003	0.47719
H	4.71157	-1.31236	0.62305
C	3.03765	-0.06612	1.43281
H	2.96255	-0.72405	2.30713
H	3.56591	0.84217	1.7371
C	1.59942	0.28137	0.92063
H	0.84114	-0.17797	1.59116
Ni	-0.13627	-0.26136	-0.18124
C	-1.9948	-0.13125	-0.06495
C	-4.16475	0.68138	-0.07567
C	-4.24117	-0.66832	0.15222
H	-4.94499	1.4216	-0.15341
H	-5.09835	-1.30295	0.31087
N	-2.92279	-1.15039	0.15494
N	-2.80307	0.99649	-0.20188
C	-2.55391	-2.55084	0.36777
H	-1.47408	-2.63625	0.22095
H	-2.80502	-2.87282	1.38654
H	-3.0676	-3.19973	-0.35233
C	-2.2937	2.34244	-0.49111
H	-1.24127	2.39656	-0.2098
H	-2.38881	2.57388	-1.55959
H	-2.85187	3.0863	0.08867
F	1.3368	1.67268	0.81249

D5

E= -845.9874049
ZPE= 0.273968
$\mathbf{H}_{corr}$ 0.291597
$\mathbf{G}_{corr}$= 0.226653
$\mathbf{E}_{tot}$= -845.713437
$\mathbf{H}_{tot}$= -845.695808
$\mathbf{G}_{tot}$= -845.7607519

C	3.8869	-1.03969	0.35357
C	4.26855	-0.12689	-0.81651
C	3.12255	0.23242	-1.44747
C	1.96619	-0.45341	-0.71593
C	2.651	-1.77113	-0.25007
H	5.27105	0.23406	-1.02032
H	3.00035	0.94405	-2.25596
H	1.03566	-0.56327	-1.3254
H	2.90961	-2.42002	-1.09219
H	2.06566	-2.3334	0.48722
H	4.68578	-1.66089	0.76408
C	3.17651	-0.12895	1.4253
H	2.95374	-0.69738	2.33567
H	3.77868	0.74181	1.69859
C	1.8337	0.29694	0.70033
H	0.96695	-0.11007	1.30239
Ni	-0.32785	-0.16405	-0.08131
C	-2.14657	-0.12248	-0.04501
C	-4.33189	0.65092	-0.08068
C	-4.38723	-0.70964	0.07805
H	-5.12549	1.37811	-0.1465
H	-5.23664	-1.36639	0.17835
N	-3.0605	-1.16965	0.09651
N	-2.97404	0.99855	-0.15086
C	-2.66708	-2.56937	0.2584
H	-1.58512	-2.62682	0.11212
H	-2.91253	-2.9339	1.26436
H	-3.16746	-3.20089	-0.48632
C	-2.47431	2.36414	-0.33607
H	-1.39483	2.36049	-0.16973
H	-2.67573	2.72077	-1.35429
H	-2.94377	3.04447	0.3844
F	1.6605	1.68244	0.59836

1-5

E= -371.9228834
ZPE= 0.144315
$\mathbf{H}_{corr}$ = 0.151874
$\mathbf{G}_{corr}$= 0.113115
$\mathbf{E}_{tot}$= -371.778569
$\mathbf{H}_{tot}$= -371.77101
$\mathbf{G}_{tot}$= -371.8097684

C	-0.65755	0.85457	0.5805
C	-0.09067	-0.61521	0.50634
C	-1.23324	-1.41501	-0.08102
C	-2.34501	-0.66421	-0.2519
C	-2.16404	0.77881	0.2075
H	0.33058	-1.05034	1.41835
H	-1.14634	-2.47037	-0.32639

H	-3.28496	-1.03253	-0.65623
H	-2.81494	1.00027	1.06596
H	-2.42826	1.50035	-0.5801
H	-0.48477	1.37428	1.52713
C	0.33877	1.2891	-0.5491
H	-0.14489	1.5273	-1.50232
H	1.01891	2.10273	-0.28373
C	1.00469	-0.1447	-0.54668
H	0.93093	-0.66711	-1.50689
F	2.35024	-0.193	-0.0955
C	2.01817	2.44096	0.39016
H	0.9467	2.45065	0.18321
H	2.20001	2.83771	1.39478
H	2.53442	3.06889	-0.34445
C	2.10613	-2.41595	-0.37577
H	1.08346	-2.37204	-0.75474
H	2.76199	-2.83233	-1.14787
H	2.13732	-3.06042	0.50983
O	-3.37132	-2.40576	1.82791
H	-2.91859	-3.14601	2.2386

A6

E= -821.9776908
ZPE= 0.285025
$\mathbf{H}_{corr}$ = 0.303216
$\mathbf{G}_{corr}$= 0.236512
$\mathbf{E}_{tot}$= -821.692665
$\mathbf{H}_{tot}$= -821.674475
$\mathbf{G}_{tot}$= -821.741178

C	-3.24027	0.41031	0.66801
C	-2.97752	-0.91917	-0.11733
C	-1.99574	-0.5023	-1.20339
C	-1.84487	0.89125	-1.24821
C	-2.70282	1.57592	-0.18915
H	-3.84627	-1.43419	-0.55028
H	-1.82618	-1.15413	-2.06143
H	-1.54209	1.44035	-2.14155
H	-3.52929	2.12255	-0.67053
H	-2.15355	2.31436	0.41329
H	-4.28076	0.55857	0.97446
C	-2.36088	-0.14104	1.82961
H	-1.34947	0.28166	1.81403
H	-2.76862	-0.04379	2.84205
C	-2.41477	-1.5559	1.18945
H	-1.4652	-2.09484	1.10281
Ni	-0.16502	0.06187	-0.61398
C	1.669	0.0213	-0.09396
C	3.78847	-0.69974	0.36787
C	3.76353	0.63974	0.5806
H	4.58918	-1.41632	0.47139
H	4.5398	1.31835	0.90032
N	2.47137	1.06194	0.29911
N	2.51242	-1.05943	-0.04341

TS-A6

E= -821.9298245
ZPE= 0.283286
$\mathbf{H}_{corr}$= 0.301119
$\mathbf{G}_{corr}$= 0.2373
$\mathbf{E}_{tot}$= -821.646539
$\mathbf{H}_{tot}$= -821.628706
$\mathbf{G}_{tot}$= -821.692525

one imaginary frequency = -406.27cm^{-1}

C	2.87874	-0.65312	0.45273
C	2.43895	0.41993	-0.58291
C	1.81453	-0.26489	-1.71658
C	1.40119	-1.56003	-1.30853
C	2.15386	-1.96682	-0.02216
H	3.06854	1.29155	-0.74954
H	1.66146	0.16854	-2.70045
H	1.01471	-2.31113	-1.99215
H	2.8812	-2.76574	-0.23896
H	1.48836	-2.35595	0.76359
H	3.9647	-0.80505	0.49166
C	2.29683	0.06968	1.69902
H	1.63162	-0.56088	2.30481
H	3.07688	0.47968	2.35606
C	1.53592	1.199	0.94808
H	0.51702	1.37032	1.31487
Ni	0.23363	0.03871	-0.53754
C	-1.57822	-0.02383	-0.03441
C	-3.80975	0.59295	0.15886
C	-3.70396	-0.69679	0.61132
H	-4.67243	1.23451	0.07473
H	-4.45735	-1.36432	0.9981

N	-2.35267	-1.06033	0.48721
N	-2.51817	0.99454	-0.21978
C	-1.80132	-2.36601	0.85135
H	-0.87162	-2.50431	0.29498
H	-1.58877	-2.42356	1.92693
H	-2.50624	-3.16142	0.58344
C	-2.18407	2.29536	-0.80282
H	-1.10034	2.43187	-0.73914
H	-2.48018	2.34394	-1.8585
H	-2.68456	3.10098	-0.25244
O	2.24112	2.49067	0.91902
H	2.28695	2.82841	-0.00248
N	2.35165	-0.86976	-0.16549
C	1.34636	2.50421	0.36951
H	0.46556	2.5426	-0.27116
H	1.03724	2.63097	1.41289
H	2.03287	3.31109	0.09847
C	2.13696	-2.27542	-0.47734
H	1.09674	-2.51176	-0.24257
H	2.32574	-2.47515	-1.53799
H	2.80608	-2.89259	0.12961
O	-1.16148	-2.69005	1.27871
H	-1.18969	-3.0885	2.15166

B6

E= -821.9681135
ZPE= 0.284328
$\mathbf{H}_{corr}$ = 0.302021
$\mathbf{G}_{corr}$= 0.240287
$\mathbf{E}_{tot}$= -821.683786
$\mathbf{H}_{tot}$= -821.666092
$\mathbf{G}_{tot}$= -821.727826

C	-2.82003	0.08823	0.62232
C	-2.46943	-0.81242	-0.56688
C	-2.05823	-0.04398	-1.68356
C	-1.66105	1.22282	-1.24534
C	-2.30014	1.49547	0.12262
H	-2.82055	-1.83655	-0.63766
H	-1.89295	-0.43334	-2.68467
H	-1.31778	2.01512	-1.90391
H	-3.13073	2.21076	0.01885
H	-1.60156	1.93955	0.84477
H	-3.90515	0.14681	0.8076
C	-2.0818	-0.48405	1.86449
H	-1.78349	0.33781	2.53059
H	-2.77424	-1.10837	2.453
C	-0.83779	-1.30226	1.39767
H	-0.00477	-1.21811	2.10677
Ni	-0.49589	-0.38382	-0.32733
C	1.34606	0.05923	-0.11974
C	3.59078	-0.29988	0.08676
C	3.37215	1.02004	0.30807
H	4.50443	-0.87441	0.08114
H	4.0549	1.82052	0.54851
N	2.00489	1.22359	0.17019

TS-B6

E= -821.9476285
ZPE= 0.28448
$\mathbf{H}_{corr}$= 0.301553
$\mathbf{G}_{corr}$= 0.24048
$\mathbf{E}_{tot}$= -821.663148
$\mathbf{H}_{tot}$= -821.646075
$\mathbf{G}_{tot}$= -821.707148

one imaginary frequency = -182.19cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033
C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-3.44835	-1.46956	1.41438
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654
H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	0.19853	0.97206	1.98788
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549

H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995
H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
O	-0.74827	-0.81864	2.31478
H	-0.74481	-0.5928	3.24783

C6

E= -821.9768186
ZPE= 0.285716
$\mathbf{H}_{corr}$ = 0.30303
$\mathbf{G}_{corr}$= 0.241186
$\mathbf{E}_{tot}$= -821.691103
$\mathbf{H}_{tot}$= -821.673789
$\mathbf{G}_{tot}$= -821.735633

C	-3.4106	0.60873	0.32478
C	-3.57856	-0.88781	0.08256
C	-2.70357	-1.28125	-0.88859
C	-1.92257	-0.11405	-1.38732
C	-2.83849	1.07804	-1.04289
H	-4.21159	-1.53494	0.68405
H	-2.54371	-2.3076	-1.21518
H	-1.5636	-0.17347	-2.4379
H	-3.6593	1.17642	-1.77493
H	-2.31591	2.04134	-0.9745
H	-4.34579	1.11635	0.59987
C	-2.34017	0.91278	1.44194
H	-2.25655	2.00926	1.50278
H	-2.76073	0.5772	2.40567
C	-0.93382	0.30465	1.25804
H	-0.17875	1.03224	1.60299
Ni	-0.19117	-0.00651	-0.54674
C	1.76088	0.02769	-0.2049
C	3.96271	-0.60204	0.12237
C	3.92055	0.76929	0.16328
H	4.79485	-1.27886	0.23281
H	4.71002	1.48794	0.31503
N	2.58163	1.13484	-0.04043
N	2.64754	-1.03568	-0.10307
C	2.08956	2.51752	-0.07618
H	1.01719	2.48516	-0.28235
H	2.25701	3.01347	0.88715
H	2.59336	3.08464	-0.86771
C	2.23907	-2.44162	-0.20872
H	1.15432	-2.46777	-0.33714
H	2.71798	-2.92042	-1.07098
H	2.50471	-2.98941	0.70282
O	-0.76398	-0.92529	1.96748
H	-0.9158	-0.77864	2.90399

TS-C6

E= -821.9349105
ZPE= 0.283782
$\mathbf{H}_{corr}$= 0.301001
$\mathbf{G}_{corr}$= 0.238693
$\mathbf{E}_{tot}$= -821.651129
$\mathbf{H}_{tot}$= -821.633909
$\mathbf{G}_{tot}$= -821.696217

one imaginary frequency = -362.09 cm^{-1}

C	3.84554	-0.57717	0.11783
C	4.01579	0.87636	-0.27487
C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	4.89943	1.47283	-0.06965
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	0.83076	-0.55465	1.67022
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335

H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
O	1.5785	1.38127	1.64983
H	1.88203	1.41806	2.55984
H	4.92449	1.54863	-0.20392
N	2.80218	1.12095	-0.07971
N	2.93219	-1.02919	0.02537
C	2.27791	2.47183	-0.15897
H	1.21875	2.42597	0.10241
H	2.80346	3.12644	0.54529
H	2.38099	2.8787	-1.17235
C	2.57753	-2.43279	0.12484
H	1.48723	-2.49007	0.13995
H	2.96095	-2.99225	-0.7365
H	2.97785	-2.87367	1.04557
O	-1.89296	-1.6101	1.49366
H	-1.15436	-1.66993	2.10398

D6

E= -821.9528019
ZPE= 0.286303
$\mathbf{H}_{corr}$ = 0.30413
$\mathbf{G}_{corr}$= 0.238499
$\mathbf{E}_{tot}$= -821.666499
$\mathbf{H}_{tot}$= -821.648672
$\mathbf{G}_{tot}$= -821.714303

C	-4.04126	0.70777	0.06248
C	-4.37008	-0.64916	-0.54484
C	-3.214	-1.2157	-0.92067
C	-2.09712	-0.24046	-0.57892
C	-2.82129	1.10829	-0.79872
H	-5.35697	-1.10172	-0.55373
H	-3.05803	-2.22327	-1.29334
H	-1.16241	-0.39221	-1.17281
H	-3.07472	1.27983	-1.84947
H	-2.26655	1.96762	-0.40397
H	-4.86531	1.42256	0.12885
C	-3.32556	0.42555	1.42801
H	-3.12639	1.3668	1.95284
H	-3.92612	-0.20529	2.08973
C	-1.99463	-0.273	0.99694
H	-1.12497	0.3033	1.4057
Ni	0.19964	-0.10871	0.08665
C	2.00683	-0.00421	0.01204
C	4.23369	-0.55286	-0.05884
C	4.15169	0.79847	-0.12843
H	5.09203	-1.20775	-0.05591

1-6

E= -347.8815146
ZPE= 0.155932
$\mathbf{H}_{corr}$ = 0.163926
$\mathbf{G}_{corr}$= 0.124363
$\mathbf{E}_{tot}$= -347.725583
$\mathbf{H}_{tot}$= -347.717589
$\mathbf{G}_{tot}$= -347.757152

C	-0.18783	-0.80949	0.57258
C	-0.3781	0.7581	0.63845
C	0.85414	1.28263	-0.07204
C	1.72819	0.29949	-0.3872
C	1.25617	-1.07851	0.06872
H	-0.52543	1.22079	1.62262
H	0.99869	2.33779	-0.29411
H	2.67575	0.45146	-0.89981
H	1.90982	-1.47509	0.86103
H	1.27134	-1.81468	-0.74939
H	-0.42464	-1.34962	1.49504
C	-1.33823	-0.87747	-0.49571
H	-0.96272	-1.0677	-1.50788
H	-2.14394	-1.5887	-0.28452
C	-1.68006	0.63201	-0.23626
H	-1.72512	1.26066	-1.10093
O	-2.87745	0.81129	0.52468
H	-3.5128	1.31316	0.00889

2-6

E= -347.8886138
ZPE= 0.157408
$\mathbf{H}_{corr}$ = 0.16481
$\mathbf{G}_{corr}$= 0.127222
$\mathbf{E}_{tot}$= -347.731206
$\mathbf{H}_{tot}$= -347.723803
$\mathbf{G}_{tot}$= -347.761392

C	-0.08784	-1.13781	0.32395
C	-1.28896	-0.67849	-0.51196
C	-1.28889	0.67866	-0.5119
C	-0.0877	1.13776	0.32407
C	-0.03905	-0.00011	1.39044
H	-1.94331	-1.3387	-1.07286
H	-1.94296	1.33932	-1.07258
H	-0.11891	2.16699	0.68974
H	-0.90918	-0.00011	2.05524
H	0.88406	-0.00019	1.98484
H	-0.11913	-2.16709	0.68946
C	1.20038	-0.78595	-0.52016
H	2.09804	-1.18453	-0.03039
H	1.15122	-1.20753	-1.52983
C	1.20049	0.78591	-0.52006
H	2.09819	1.18431	-0.0302
O	1.1364	1.33657	-1.83823
H	1.94848	1.81268	-2.02647
H	-1.13778	-0.54616	2.58577
H	-0.05494	-2.76754	1.69289
H	-1.90825	-3.5801	0.13734
H	-0.76582	-2.86296	-1.00203
H	-3.44337	-1.94783	-0.68888
C	-2.05351	-0.39457	-1.46139
H	-1.01855	-0.45719	-1.81265
H	-2.72877	-0.25147	-2.30934
C	-2.20183	0.67332	-0.32986
H	-1.35902	1.33594	-0.1414
Ni	0.59173	-0.5594	0.71943
C	2.2246	0.18125	0.06886
C	3.96669	1.64144	-0.36196
C	4.2575	0.46254	-0.99886
H	4.51958	2.56601	-0.31645
H	5.10888	0.18425	-1.59908
N	3.19317	-0.41367	-0.73093
N	2.73378	1.45687	0.28419
C	3.10718	-1.79338	-1.21894
H	2.16522	-2.21763	-0.86334
H	3.12293	-1.8182	-2.31527
H	3.93872	-2.39449	-0.83185
C	2.05199	2.4792	1.0854
H	1.19838	2.01091	1.58219
H	2.72919	2.88314	1.84689
H	1.69045	3.29818	0.45197
C	-3.43403	1.58364	-0.48665
N	-4.36219	2.26933	-0.60475

A7

E= -838.9913325
ZPE= 0.280118
$\mathbf{H}_{corr}$ = 0.298745
$\mathbf{G}_{corr}$= 0.231072
$\mathbf{E}_{tot}$= -838.711214
$\mathbf{H}_{tot}$= -838.693532
$\mathbf{G}_{tot}$= -838.760261

C	-2.45414	-1.53868	-0.46713
C	-2.42635	-0.49562	0.71576
C	-1.21073	-0.8797	1.5501
C	-0.63309	-2.08653	1.06569
C	-1.40934	-2.63759	-0.13812
H	-3.34086	-0.37975	1.30861

TS-A7

E= -838.9514662
ZPE= 0.278063
$\mathbf{H}_{corr}$= 0.296415
$\mathbf{G}_{corr}$= 0.230746
$\mathbf{E}_{tot}$= -838.673403
$\mathbf{H}_{tot}$= -838.655996
$\mathbf{G}_{tot}$= -838.72072

one imaginary frequency = -383.74 cm^{-1}

C	-2.55254	-1.55327	-0.46948
C	-2.29234	-0.65671	0.75989
C	-1.33155	-1.2935	1.63083
C	-0.59466	-2.26845	0.86922

C	-1.34134	-2.55768	-0.45517
H	-3.09206	-0.02596	1.14716
H	-1.2252	-1.09476	2.69256
H	0.01502	-3.03997	1.3343
H	-1.69075	-3.60043	-0.48619
H	-0.70118	-2.41487	-1.33832
H	-3.49851	-2.10533	-0.39806
C	-2.54861	-0.4296	-1.53714
H	-2.06142	-0.69089	-2.48405
H	-3.56129	-0.07096	-1.74713
C	-1.77556	0.62697	-0.73678
H	-0.7285	0.78935	-0.99427
Ni	0.15494	-0.40687	0.6264
C	1.89345	0.10069	0.04352
C	3.7703	1.40553	-0.27766
C	4.08637	0.13269	-0.67918
H	4.36681	2.30342	-0.26636
H	5.00262	-0.2663	-1.08344
N	2.93801	-0.64926	-0.4768
N	2.43563	1.37575	0.152
C	2.84642	-2.07953	-0.78409
H	1.88902	-2.44395	-0.4087
H	2.90088	-2.25018	-1.86625
H	3.65854	-2.62819	-0.29289
C	1.71108	2.53511	0.70129
H	0.64281	2.46137	0.47533
H	1.84692	2.59498	1.78776
H	2.09215	3.45358	0.24297
C	-2.43488	1.97102	-0.37561
N	-2.93152	2.98341	-0.10357

C	-1.36629	-2.52025	-0.33783
H	-2.87195	0.15195	1.28973
H	-1.20336	-1.2328	2.86324
H	0.12757	-2.99283	1.37357
H	-1.86918	-3.49959	-0.31578
H	-0.71024	-2.52107	-1.21858
H	-3.43397	-1.74561	-0.5244
C	-2.15389	-0.26438	-1.51124
H	-1.76885	-0.74055	-2.42393
H	-3.10043	0.23044	-1.76838
C	-1.13804	0.80416	-1.02665
H	-0.35168	1.06962	-1.73544
Ni	-0.24625	-0.27195	0.45181
C	1.62277	-0.047	0.0959
C	3.64832	1.04791	0.06001
C	3.82926	-0.159	-0.56511
H	4.34419	1.84845	0.25054
H	4.7067	-0.59041	-1.01844
N	2.58789	-0.81705	-0.53069
N	2.30403	1.1045	0.45123
C	2.34416	-2.13171	-1.13161
H	1.54643	-2.63136	-0.5824
H	2.04834	-2.03377	-2.18322
H	3.25374	-2.7383	-1.07314
C	1.68318	2.24032	1.16005
H	0.76247	2.5424	0.65014
H	1.46438	1.96716	2.19836
H	2.37837	3.08565	1.15454
C	-1.76888	2.12194	-0.53973
N	-2.24406	3.11455	-0.17295

B7

E= -838.9984554
ZPE= 0.279554
$\mathbf{H}_{corr}$ = 0.298024
$\mathbf{G}_{corr}$= 0.232872
$\mathbf{E}_{tot}$= -838.718901
$\mathbf{H}_{tot}$= -838.701375
$\mathbf{G}_{tot}$= -838.765584

C	-2.41958	-1.33725	-0.40545
C	-2.22836	-0.65698	0.96361
C	-1.37632	-1.41862	1.80823
C	-0.60533	-2.28975	0.98838

TS-B7

E= -838.9572652
ZPE= 0.278623
$\mathbf{H}_{corr}$= 0.29665
$\mathbf{G}_{corr}$= 0.232637
$\mathbf{E}_{tot}$= -838.678643
$\mathbf{H}_{tot}$= -838.660615
$\mathbf{G}_{tot}$= -838.724628

one imaginary frequency = -373.32 cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033

C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-3.44835	-1.46956	1.41438
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654
H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	0.19853	0.97206	1.98788
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549
H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995
H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
C	-0.75996	-0.91012	2.37475
N	-0.88327	-1.87476	3.0071
C	2.00875	0.60011	-1.06473
C	2.86564	-0.66987	-1.10316
H	4.24159	1.16354	1.41048
H	2.69264	2.57668	-0.16316
H	1.71139	1.01621	-2.05005
H	3.7166	-0.55709	-1.79483
H	2.32101	-1.58255	-1.37841
H	4.27961	-1.32544	0.47557
C	2.25143	-1.25223	1.27174
H	2.0473	-2.29128	0.97184
H	2.64141	-1.30459	2.30078
C	0.95569	-0.44483	1.25667
H	0.13706	-1.02564	1.70279
Ni	0.23753	0.2524	-0.40606
C	-1.72097	0.05051	-0.13083
C	-3.91749	0.47413	0.31565
C	-3.79496	-0.86404	0.11842
H	-4.78102	1.07723	0.55222
H	-4.53153	-1.65263	0.15002
N	-2.45627	-1.10083	-0.15372
N	-2.64864	1.01165	0.15956
C	-1.88896	-2.41513	-0.42771
H	-0.81029	-2.29206	-0.53394
H	-2.09974	-3.09986	0.39982
H	-2.30491	-2.82723	-1.35301
C	-2.32977	2.4262	0.3014
H	-1.24424	2.52791	0.25218
H	-2.78985	3.01008	-0.5028
H	-2.68497	2.79932	1.26711
C	1.11264	0.87113	2.04103
N	1.23086	1.86237	2.63184

C7

E= -838.9912407
ZPE= 0.279308
$\mathbf{H}_{corr}$ = 0.297758
$\mathbf{G}_{corr}$= 0.232338
$\mathbf{E}_{tot}$= -838.711933
$\mathbf{H}_{tot}$= -838.694427
$\mathbf{G}_{tot}$= -838.758902

C	3.38544	-0.70088	0.35188
C	3.62143	0.7761	0.60668
C	2.8094	1.49501	-0.19498

TS-C7

E= -838.9494197
ZPE= 0.278167
$\mathbf{H}_{corr}$= 0.296249
$\mathbf{G}_{corr}$= 0.231002
$\mathbf{E}_{tot}$= -838.671252
$\mathbf{H}_{tot}$= -838.653171
$\mathbf{G}_{tot}$= -838.718418

one imaginary frequency = -338.34 cm^{-1}

C	3.84554	-0.57717	0.11783

C	4.01579	0.87636	-0.27487
C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	4.89943	1.47283	-0.06965
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	0.83076	-0.55465	1.67022
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335
H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
C	1.57425	1.48514	1.68578
N	1.52952	2.58053	2.0649

D7

E= -838.9586646
ZPE= 0.28011
$\mathbf{H}_{corr}$ = 0.298748
$\mathbf{G}_{corr}$= 0.23086
$\mathbf{E}_{tot}$= -838.678555
$\mathbf{H}_{tot}$= -838.660861
$\mathbf{G}_{tot}$= -838.727804

C	-4.03782	0.72418	0.11839
C	-4.39757	-0.58528	-0.59416
C	-3.23807	-1.15089	-1.01632
C	-2.096	-0.21918	-0.59797
C	-2.79874	1.16647	-0.71702
H	-5.39571	-1.00786	-0.65135
H	-3.10056	-2.1227	-1.47963
H	-1.16457	-0.34852	-1.20239
H	-3.05046	1.4212	-1.75171
H	-2.22922	1.98356	-0.25792
H	-4.84792	1.44762	0.23715
C	-3.32441	0.32402	1.46785
H	-3.10906	1.22204	2.06045
H	-3.94017	-0.34608	2.07694
C	-1.99954	-0.37104	0.98474
H	-1.11825	0.15237	1.44268
Ni	0.19474	-0.12982	0.0835
C	1.99943	-0.00379	0.00641
C	4.26193	-0.53603	-0.05646
C	4.16611	0.82954	-0.12307
H	5.13128	-1.17438	-0.05763
H	4.93794	1.57957	-0.19365
N	2.79819	1.14425	-0.08358
N	2.95077	-1.0329	0.02093
C	2.25404	2.50012	-0.1402
H	1.16798	2.42181	-0.03888
H	2.64985	3.11514	0.67838
H	2.49063	2.98005	-1.0989
C	2.60073	-2.44963	0.11036
H	1.50923	-2.51801	0.10957
H	2.99749	-3.00572	-0.74889
H	2.98747	-2.89371	1.037
C	-1.93263	-1.85076	1.4061
N	-1.88223	-2.96536	1.72348

1-7

E= -364.8923202
ZPE= 0.151075
$\mathbf{H}_{corr}$ = 0.159524
$\mathbf{G}_{corr}$= 0.118366
$\mathbf{E}_{tot}$= -364.741245
$\mathbf{H}_{tot}$= -364.73374
$\mathbf{G}_{tot}$= -364.773955

C	-0.3339	0.85771	0.56789
C	0.14444	-0.64772	0.52895

C	-1.02616	-1.37448	-0.09817
C	-2.08543	-0.55975	-0.30758
C	-1.83277	0.8702	0.16074
H	0.51587	-1.10465	1.4523
H	-0.99629	-2.43363	-0.34321
H	-3.03086	-0.87057	-0.74679
H	-2.48965	1.12511	1.00609
H	-2.03838	1.60844	-0.62946
H	-0.14222	1.38617	1.50554
C	0.71274	1.1886	-0.55611
H	0.25249	1.40446	-1.52769
H	1.42564	1.98312	-0.30984
C	1.3015	-0.26069	-0.44487
H	1.34991	-0.82774	-1.38521
C	2.64248	-0.35002	0.30706
N	3.65257	-0.41731	0.87344

2-7

E= -364.9003212
ZPE= 0.152442
$\mathbf{H}_{corr}$ = 0.160263
$\mathbf{G}_{corr}$= 0.121169
$\mathbf{E}_{tot}$= -364.747879
$\mathbf{H}_{tot}$= -364.741002
$\mathbf{G}_{tot}$= -364.779152

C	-1.20596	-0.7293	-0.42397
C	-1.21471	0.69309	-0.99593
C	-0.47009	1.46813	-0.16931
C	0.02473	0.57719	0.97615
C	-1.17503	-0.41191	1.10566
H	-1.64751	0.97317	-1.95099
H	-0.16843	2.49784	-0.32039
H	0.36253	1.09023	1.87839
H	-2.08763	0.07665	1.46023
H	-0.9585	-1.28938	1.73026
H	-1.98972	-1.4005	-0.78297
C	0.26329	-1.27525	-0.62348
H	0.32539	-2.34073	-0.36708
H	0.60581	-1.14075	-1.65561
C	1.09651	-0.39217	0.37199
H	1.52362	-1.01196	1.17571
C	2.21868	0.43767	-0.27894
N	3.06395	1.06275	-0.76925

A8

E= -878.3015628
ZPE= 0.307894
$\mathbf{H}_{corr}$ = 0.328054
$\mathbf{G}_{corr}$= 0.257611
$\mathbf{E}_{tot}$= -877.993669
$\mathbf{H}_{tot}$= -877.973509
$\mathbf{G}_{tot}$= -878.043952

C	2.77786	-1.20152	0.5558
C	2.71996	-0.15976	-0.62663
C	1.55421	-0.62694	-1.49285
C	1.05979	-1.87914	-1.03771
C	1.84379	-2.38316	0.18156
H	1.47581	-0.28623	-2.52612
H	0.54343	-2.59242	-1.68296
H	2.43067	-3.27461	-0.09163
H	1.19732	-2.67589	1.02279
H	3.78654	-1.5357	0.82012
C	2.24187	-0.10409	1.53716
H	1.18832	-0.24447	1.802
H	2.83127	0.05743	2.44416
C	2.40966	0.9982	0.41816
H	1.48538	1.54217	0.19246
Ni	-0.29272	-0.45703	-0.70336
C	-1.99274	0.13958	-0.0851
C	-3.86347	1.43499	0.33911
C	-4.07158	0.21517	0.92939
H	-4.49042	2.31164	0.30681
H	-4.91267	-0.15259	1.49503
N	-2.93058	-0.56016	0.66641
N	-2.60191	1.3754	-0.27512
C	-2.74393	-1.94462	1.11044
H	-1.74569	-2.2646	0.80197
H	-2.82427	-2.01482	2.20191
H	-3.48891	-2.60476	0.64984
C	-1.98823	2.47655	-1.02396
H	-1.07543	2.10187	-1.49403
H	-2.66862	2.83562	-1.80505
H	-1.73219	3.30931	-0.35758
C	3.4955	1.95332	0.64057
N	4.37571	2.72387	0.81497
C	4.0086	0.0645	-1.43947
H	3.95016	1.00373	-1.94873
H	4.8506	0.06856	-0.77922

H	4.1204	-0.72296	-2.15523

TS-A8

E= -878.2623685
ZPE= 0.305636
$\mathbf{H}_{corr}$= 0.325638
$\mathbf{G}_{corr}$= 0.256598
$\mathbf{E}_{tot}$= -877.956732
$\mathbf{H}_{tot}$= -877.93673
$\mathbf{G}_{tot}$= -878.005771

one imaginary frequency = -344.79 cm^{-1}

C	-2.80552	-1.11489	-0.39988
C	-2.44734	-0.12854	0.73635
C	-1.60709	-0.81273	1.70653
C	-1.00974	-1.95183	1.083
C	-1.77426	-2.29052	-0.21834
H	-1.46837	-0.50545	2.73831
H	-0.48864	-2.7275	1.63821
H	-2.28853	-3.25971	-0.12795
H	-1.1125	-2.36873	-1.09443
H	-3.83068	-1.50072	-0.32397
C	-2.58073	-0.14293	-1.58413
H	-2.02875	-0.57717	-2.42702
H	-3.5232	0.26078	-1.97248
C	-1.76049	0.9523	-0.83075
H	-0.71424	1.00759	-1.15302
Ni	-0.09282	-0.17892	0.56791
C	1.70486	0.05129	0.0287
C	3.8085	1.00131	-0.18047
C	3.88574	-0.27263	-0.68056
H	4.56555	1.76386	-0.09097
H	4.7197	-0.80551	-1.10841
N	2.60706	-0.83835	-0.54629
N	2.48197	1.18983	0.23903
C	2.2518	-2.19577	-0.9662
H	1.30438	-2.45761	-0.49172
H	2.13933	-2.25543	-2.05624
H	3.02377	-2.90523	-0.64653
C	1.97421	2.41313	0.868
H	0.88116	2.38712	0.85255
H	2.30835	2.48772	1.91011
H	2.3154	3.2957	0.3154
C	-2.31876	2.27062	-0.71263
N	-2.79568	3.34805	-0.55406
C	-3.49012	0.90283	1.20591
H	-4.12065	1.17191	0.38436
H	-4.08466	0.47834	1.98772
H	-2.98958	1.77485	1.57188

B8

E= -878.3100954
ZPE= 0.307371
$\mathbf{H}_{corr}$ = 0.327533
$\mathbf{G}_{corr}$= 0.259498
$\mathbf{E}_{tot}$= -878.002724
$\mathbf{H}_{tot}$= -877.982562
$\mathbf{G}_{tot}$= -878.050597

C	2.49906	-1.02131	0.57865
C	2.30253	-0.25869	-0.75127
C	1.5765	-1.06838	-1.67731
C	0.86533	-2.06599	-0.96536
C	1.54571	-2.27519	0.40761
H	1.4533	-0.84433	-2.73292
H	0.24444	-2.82298	-1.43533
H	2.12017	-3.21462	0.40606
H	0.82848	-2.34409	1.23777
H	3.54287	-1.35948	0.70233
C	2.12273	-0.05684	1.7398
H	1.91273	-0.62557	2.65782
H	2.98342	0.58945	1.96509
C	0.86924	0.81756	1.35104
H	0.04713	0.68373	2.06484
Ni	0.25422	-0.13071	-0.32817
C	-1.64535	-0.08021	-0.14653
C	-3.75289	0.8576	-0.22554
C	-3.88628	-0.39568	0.31293
H	-4.49376	1.61291	-0.43175
H	-4.7612	-0.91807	0.66444
N	-2.5973	-0.95609	0.35045
N	-2.38794	1.03929	-0.49382
C	-2.2934	-2.28165	0.89589
H	-1.37238	-2.64496	0.43969
H	-2.16061	-2.23799	1.98397
H	-3.10828	-2.97558	0.66344
C	-1.81162	2.24878	-1.10084
H	-0.76894	2.3431	-0.79044

H	-1.8615	2.1956	-2.19513
H	-2.35879	3.13188	-0.75593
C	1.11153	2.22855	1.17704
N	1.28227	3.39096	0.9795
C	3.2004	0.88683	-1.15031
H	3.17051	1.71264	-0.43166
H	4.24865	0.55043	-1.22299
H	2.91529	1.29629	-2.12817

TS-B8

E= -878.2695898
ZPE= 0.306646
$\mathbf{H}_{corr}$= 0.326295
$\mathbf{G}_{corr}$= 0.259051
$\mathbf{E}_{tot}$= -877.962944
$\mathbf{H}_{tot}$= -877.943295
$\mathbf{G}_{tot}$= -878.010539

one imaginary frequency = -418.84 cm^{-1}

C	-3.01465	0.60162	0.48584
C	-3.08773	-0.91857	0.55033
C	-2.48115	-1.45605	-0.54534
C	-1.96169	-0.44549	-1.47406
C	-2.73011	0.82926	-1.03393
H	-2.34545	-2.52655	-0.69772
H	-1.97361	-0.68144	-2.5377
H	-3.69586	0.89348	-1.5654
H	-2.20367	1.77651	-1.21397
H	-3.95996	1.08405	0.77335
C	-1.91262	1.17383	1.42647
H	-1.69571	2.20767	1.12194
H	-2.32759	1.24448	2.44743
C	-0.59627	0.37053	1.53525
H	0.19853	0.97206	1.98788
Ni	-0.34191	-0.26002	-0.25308
C	1.47413	-0.03649	-0.0771
C	3.69908	-0.47119	0.10465
C	3.56347	0.85909	-0.12096
H	4.58055	-1.07994	0.23549
H	4.30358	1.63846	-0.21852
N	2.20207	1.11183	-0.22753
N	2.41676	-1.00452	0.13998
C	1.61268	2.42202	-0.45995
H	0.60847	2.27566	-0.86113
H	1.54998	2.99562	0.47104
H	2.21712	2.97431	-1.1853
C	2.1125	-2.41599	0.3229
H	1.03133	-2.51778	0.42561
H	2.44782	-2.99875	-0.54197
H	2.60141	-2.79332	1.22646
C	-0.75996	-0.91012	2.37475
N	-0.88327	-1.87476	3.0071
C	-3.59893	-1.69963	1.77516
H	-4.64099	-1.91034	1.65433
H	-3.05727	-2.61813	1.86395
H	-3.45369	-1.11312	2.65823

C8

E= -878.3057377
ZPE= 0.307248
$\mathbf{H}_{corr}$= 0.32737
$\mathbf{G}_{corr}$= 0.258499
$\mathbf{E}_{tot}$= -877.99849
$\mathbf{H}_{tot}$= -877.978368
$\mathbf{G}_{tot}$= -878.047239

C	3.38544	-0.70088	0.35188
C	3.62143	0.7761	0.60668
C	2.8094	1.49501	-0.19498
C	2.00875	0.60011	-1.06473
C	2.86564	-0.66987	-1.10316
H	2.69264	2.57668	-0.16316
H	1.71139	1.01621	-2.05005
H	3.7166	-0.55709	-1.79483
H	2.32101	-1.58255	-1.37841
H	4.27961	-1.32544	0.47557
C	2.25143	-1.25223	1.27174
H	2.0473	-2.29128	0.97184
H	2.64141	-1.30459	2.30078
C	0.95569	-0.44483	1.25667
H	0.13706	-1.02564	1.70279
Ni	0.23753	0.2524	-0.40606
C	-1.72097	0.05051	-0.13083
C	-3.91749	0.47413	0.31565
C	-3.79496	-0.86404	0.11842
H	-4.78102	1.07723	0.55222
H	-4.53153	-1.65263	0.15002

N	-2.45627	-1.10083	-0.15372
N	-2.64864	1.01165	0.15956
C	-1.88896	-2.41513	-0.42771
H	-0.81029	-2.29206	-0.53394
H	-2.09974	-3.09986	0.39982
H	-2.30491	-2.82723	-1.35301
C	-2.32977	2.4262	0.3014
H	-1.24424	2.52791	0.25218
H	-2.78985	3.01008	-0.5028
H	-2.68497	2.79932	1.26711
C	1.11264	0.87113	2.04103
N	1.23086	1.86237	2.63184
C	4.50033	1.32518	1.74582
H	5.5315	1.24152	1.47273
H	4.25934	2.35332	1.91836
H	4.3208	0.76222	2.63787

TS-C8

E= -878.264704
ZPE= 0.30606
$\mathbf{H}_{corr}$= 0.325898
$\mathbf{G}_{corr}$= 0.256672
$\mathbf{E}_{tot}$= -877.958644
$\mathbf{H}_{tot}$= -877.938806
$\mathbf{G}_{tot}$= -878.008032

one imaginary frequency = -333.08 cm^{-1}

C	3.84554	-0.57717	0.11783
C	4.01579	0.87636	-0.27487
C	2.83659	1.31484	-0.75339
C	1.86991	0.17631	-0.77344
C	2.80076	-1.03594	-0.91372
H	2.57437	2.33706	-1.00946
H	1.05771	0.26497	-1.55679
H	3.22404	-1.0898	-1.92461
H	2.32718	-1.9924	-0.66674
H	4.76451	-1.16815	0.17966
C	3.00217	-0.62431	1.43747
H	2.87122	-1.67366	1.7288
H	3.52426	-0.12241	2.25919
C	1.63365	0.03093	1.18246
H	0.83076	-0.55465	1.67022
Ni	0.01297	0.04541	-0.08956
C	-1.86512	0.00461	-0.02158
C	-4.06533	0.63705	0.08751
C	-4.04096	-0.71578	-0.00675
H	-4.89475	1.32397	0.16335
H	-4.84505	-1.4357	-0.03333
N	-2.70487	-1.08486	-0.0713
N	-2.7437	1.05978	0.07492
C	-2.23765	-2.45457	-0.19601
H	-1.15196	-2.44024	-0.08306
H	-2.68098	-3.08254	0.58476
H	-2.49294	-2.8682	-1.17843
C	-2.32709	2.44836	0.16683
H	-1.23837	2.46691	0.08972
H	-2.76083	3.0362	-0.64983
H	-2.63289	2.88391	1.12512
C	1.57425	1.48514	1.68578
N	1.52952	2.58053	2.0649
C	5.2692	1.72243	0.01623
H	6.09313	1.34724	-0.55409
H	5.08274	2.74083	-0.25395
H	5.5026	1.66707	1.05899

D8

E= -878.2740192
ZPE= 0.30818
$\mathbf{H}_{corr}$= 0.328486
$\mathbf{G}_{corr}$= 0.257242
$\mathbf{E}_{tot}$= -877.96584
$\mathbf{H}_{tot}$= -877.945534
$\mathbf{G}_{tot}$= -878.016777

C	-4.03782	0.72418	0.11839
C	-4.39757	-0.58528	-0.59416
C	-3.23807	-1.15089	-1.01632
C	-2.096	-0.21918	-0.59797
C	-2.79874	1.16647	-0.71702
H	-3.10056	-2.1227	-1.47963
H	-1.16457	-0.34852	-1.20239
H	-3.05046	1.4212	-1.75171
H	-2.22922	1.98356	-0.25792
H	-4.84792	1.44762	0.23715
C	-3.32441	0.32402	1.46785
H	-3.10906	1.22204	2.06045
H	-3.94017	-0.34608	2.07694

C	-1.99954	-0.37104	0.98474
H	-1.11825	0.15237	1.44268
Ni	0.19474	-0.12982	0.0835
C	1.99943	-0.00379	0.00641
C	4.26193	-0.53603	-0.05646
C	4.16611	0.82954	-0.12307
H	5.13128	-1.17438	-0.05763
H	4.93794	1.57957	-0.19365
N	2.79819	1.14425	-0.08358
N	2.95077	-1.0329	0.02093
C	2.25404	2.50012	-0.1402
H	1.16798	2.42181	-0.03888
H	2.64985	3.11514	0.67838
H	2.49063	2.98005	-1.0989
C	2.60073	-2.44963	0.11036
H	1.50923	-2.51801	0.10957
H	2.99749	-3.00572	-0.74889
H	2.98747	-2.89371	1.037
C	-1.93263	-1.85076	1.4061
N	-1.88223	-2.96536	1.72348
C	-5.81374	-1.18484	-0.6753
H	-6.43881	-0.54505	-1.26255
H	-5.76599	-2.15218	-1.13014
H	-6.22039	-1.27386	0.3104

1-8

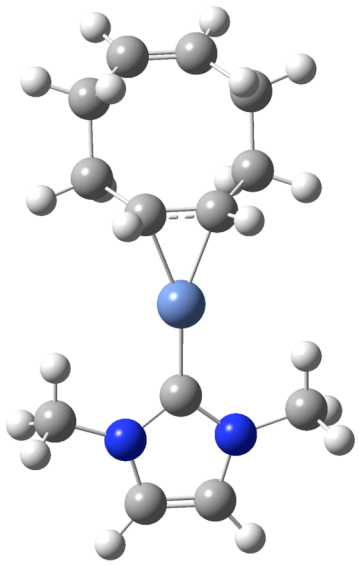
E= -404.2026682
ZPE= 0.178788
H_{corr}= 0.188761
G_{corr}= 0.144699
E_{tot}= -404.02388
H_{tot}= -404.014851
G_{tot}= -404.057969

C	-1.0251	-0.96141	-0.31267
C	-0.41623	0.4604	-0.62054
C	-1.52798	1.41971	-0.25383
C	-2.66141	0.77006	0.09652
C	-2.52599	-0.74717	0.02059
H	-1.4065	2.49918	-0.28406
H	-3.58854	1.25794	0.38768
H	-3.18519	-1.15873	-0.75742
H	-2.81227	-1.23576	0.96394
H	-0.85892	-1.71502	-1.08532
C	-0.03566	-1.09926	0.89642
H	-0.51482	-1.0566	1.87977
H	0.62992	-1.96505	0.85305
C	0.65677	0.25316	0.51974
H	0.71535	1.02473	1.28675
C	2.08911	0.08632	-0.02078
N	3.16802	-0.03935	-0.42792
C	0.19691	0.70001	-2.01275
H	0.85556	1.54229	-1.97224
H	0.74548	-0.16753	-2.31499
H	-0.5843	0.89174	-2.71833

2-8

E= -404.215692
ZPE= 0.18036
H_{corr}= 0.189866
G_{corr}= 0.146985
E_{tot}= -404.035332
H_{tot}= -404.025826
G_{tot}= -404.068707

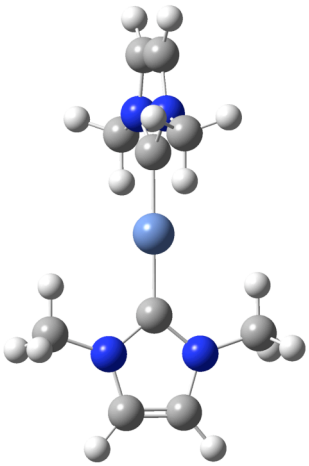
C	1.82895	-0.50009	-0.50336
C	1.56147	-0.92315	0.94399
C	0.75703	0.01412	1.50383
C	0.48709	1.08145	0.43893
C	1.8379	1.05365	-0.34233
H	0.29283	-0.00989	2.48306
H	0.10787	2.04281	0.78593
H	2.67167	1.41804	0.26446
H	1.81045	1.59479	-1.29703
H	2.68982	-0.95999	-0.9918
C	0.46842	-0.69539	-1.2848
H	0.6052	-0.53812	-2.36039
H	0.03497	-1.68518	-1.12623
C	-0.4262	0.42331	-0.68097
H	-0.72531	1.18486	-1.40535
C	-1.76105	-0.06268	-0.08634
N	-2.76653	-0.42874	0.36156
C	2.01521	-2.25532	1.56932
H	2.87413	-2.62065	1.04617
H	2.26377	-2.09991	2.59838
H	1.22299	-2.97099	1.4979



Ni(NHC)COD

E= -786.0765788
ZPE= 0.309993
$\mathbf{H}_{corr}$= 0.328803
$\mathbf{G}_{corr}$= 0.26103
$\mathbf{E}_{tot}$= -785.762472
$\mathbf{H}_{tot}$= -785.810449
$\mathbf{G}_{tot}$= -785.743818

Ni	-0.2785	0.18702	-0.43521
C	1.57702	-0.06104	-0.00868
C	3.59894	-1.00987	0.46666
C	3.77291	0.32392	0.48554
H	4.34697	-1.753	0.64861
H	4.68584	0.845	0.68538
N	2.47104	0.92718	0.1796
N	2.18702	-1.25033	0.14877
C	2.1905	2.36758	0.09329
H	1.17506	2.55078	0.37652
H	2.84578	2.89865	0.75168
H	2.34646	2.70177	-0.91115
C	1.54678	-2.56763	0.02342
H	0.74133	-2.50739	-0.67837
H	2.26559	-3.2824	-0.31911
H	1.16741	-2.87195	0.97651
C	-2.23609	-0.04237	-0.26809
C	-1.81161	1.28438	-0.12944
H	-2.02177	-0.47895	-1.22117
C	-2.98469	-0.97288	0.70276
C	-1.38702	2.07275	1.12215
H	-1.74101	1.83092	-1.04662
H	-2.31537	-1.44187	1.39338
H	-3.45035	-1.71299	0.08607
C	-4.11178	-0.24985	1.4644
C	-2.5226	2.77702	1.88669
H	-0.87954	1.43069	1.81144
H	-0.72288	2.82938	0.75975
C	-3.67845	0.54509	2.71148
H	-4.615	0.3915	0.77135
H	-4.78165	-0.99787	1.83404
C	-3.26648	1.83047	2.84852
H	-2.06493	3.5155	2.51126
H	-3.19464	3.24625	1.19887
H	-3.74477	-0.00083	3.62934
H	-3.47903	2.25915	3.80558

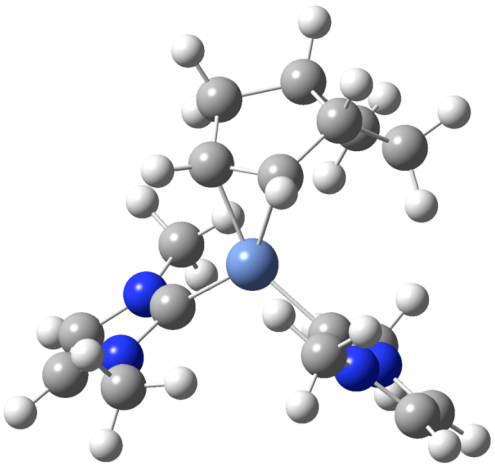


Ni(NHC)2

E= -778.8676741
ZPE= 0.25755
$\mathbf{H}_{corr}$= 0.275553
$\mathbf{G}_{corr}$= 0.210598
$\mathbf{E}_{tot}$= -778.610124
$\mathbf{H}_{tot}$= -778.657076
$\mathbf{G}_{tot}$= -778.592121

C	-0.01737	-0.00005	-0.00024
C	2.19188	-0.68545	-0.0001
C	2.19171	0.68592	-0.00016
H	3.01472	-1.38233	-0.00021
H	3.01438	1.38299	-0.00039

N	0.84914	-1.09361	-0.00013
N	0.84887	1.09375	-0.00027
C	0.39746	-2.48686	0.00043
H	-0.69599	-2.47753	-0.00331
H	0.75746	-3.01267	-0.89263
H	0.75111	-3.01009	0.89754
C	0.3969	2.48689	0.00049
H	-0.69656	2.47734	-0.00357
H	0.75019	3.00999	0.89783
H	0.75703	3.013	-0.89234
Ni	-1.93737	-0.00016	-0.00008
C	-3.85737	-0.00029	0.00005
C	-5.12648	0.67414	-1.7774
C	-5.11217	-0.69555	-1.75192
H	-5.65819	1.26337	-2.52313
H	-5.6438	-1.29097	-2.4928
C	-4.05158	2.55335	-0.28234
H	-3.72503	2.57638	0.73636
H	-3.28371	2.95165	-0.91212
H	-4.93893	3.14226	-0.38583
C	-4.0389	-2.57226	-0.24435
H	-3.27647	-2.97809	-0.87593
H	-3.70491	-2.58629	0.7721
H	-4.92815	-3.16028	-0.33574
N	-4.34962	1.09938	-0.69312
N	-4.33705	-1.12164	-0.66672

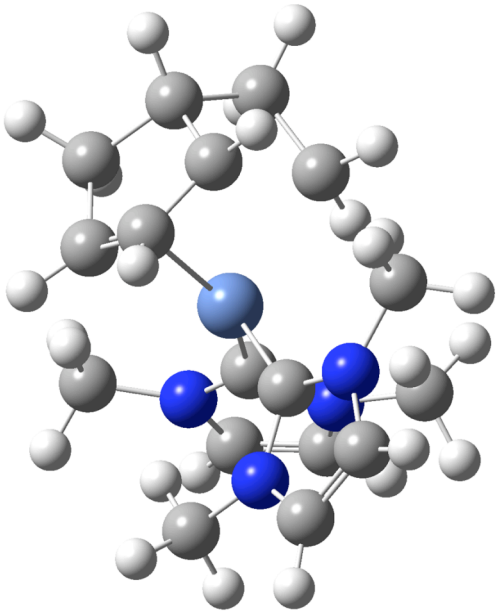


A1-dimer (B3LYP/6-31G(d)) with methyl groups to model IPr ligands

E= -1051.5513506
ZPE= 0.410966
$\mathbf{H}_{corr}$= 0.435590
$\mathbf{G}_{corr}$= 0.356624
$\mathbf{E}_{tot}$= -1051.140384
$\mathbf{H}_{tot}$= -1051.115760
$\mathbf{G}_{tot}$= -1051.194726

C	4.51568	-0.88715	0.02176
C	4.276	0.3471	-0.9342
C	3.30955	-0.19092	-1.98958
C	3.13487	-1.59224	-1.85758
C	3.95279	-2.14956	-0.68419
H	5.15893	0.80396	-1.40245
H	3.1771	0.34515	-2.93123
H	2.84526	-2.24777	-2.68151
H	4.7674	-2.78922	-1.06242
H	3.35558	-2.76891	0.00277
H	5.5539	-1.01833	0.34813
C	3.63545	-0.17809	1.11216
H	2.62391	-0.59898	1.16143
H	4.05674	-0.13468	2.12301
C	3.68507	1.1515	0.28143
H	4.3983	1.879	0.69031
H	2.72508	1.64916	0.10645
C	-0.02439	-0.47157	-0.1841
C	-1.72456	0.41324	1.11845
C	-1.70899	-0.94031	1.33627
H	-2.36031	1.17987	1.53194
H	-2.33043	-1.55267	1.97006
N	-0.67578	-1.465	0.5426
N	-0.70224	0.68482	0.19432
C	-0.31606	-2.88342	0.47121
H	0.53267	-2.97901	-0.21073
H	-0.02772	-3.26142	1.45986
H	-1.15351	-3.47854	0.08651
C	-0.37464	2.01761	-0.31862
H	0.40589	1.90577	-1.07554
H	-1.25546	2.48123	-0.77932
H	-0.00328	2.66622	0.48459
Ni	1.43639	-0.65114	-1.38159
C	0.57441	-0.86433	-3.08392
C	-0.22105	-1.78604	-4.9764
C	-0.349	-0.42599	-5.08038
H	-0.66434	-2.55763	-5.76648
H	-0.70994	0.02739	-5.94396

N	0.21766	0.1845	-4.05308
N	0.20249	-2.11038	-3.75196
C	0.3073	-3.33242	-2.94169
H	-0.26832	-4.09739	-3.41957
H	1.1486	-3.77399	-2.44961
H	-0.30099	-2.82529	-2.22218
C	0.68218	1.53538	-3.75151
H	-0.14824	2.16099	-4.00436
H	0.69228	1.36574	-2.69509
H	1.59253	2.01536	-4.04439

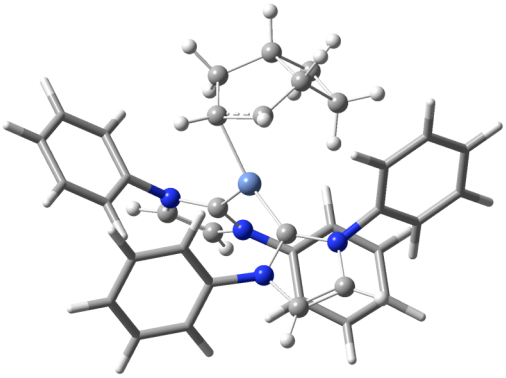


TS-A1-dimer (B3LYP/6-31G(d)) with methyl groups to model IPr ligands

one imaginary frequency = -359.70 cm^{-1}

E= -1051.4820583
ZPE= 0.408010
H$_{corr}$= 0.432663
G$_{corr}$= 0.353773
E$_{tot}$= -1051.074048
H$_{tot}$= -1051.049396
G$_{tot}$= -1051.128285

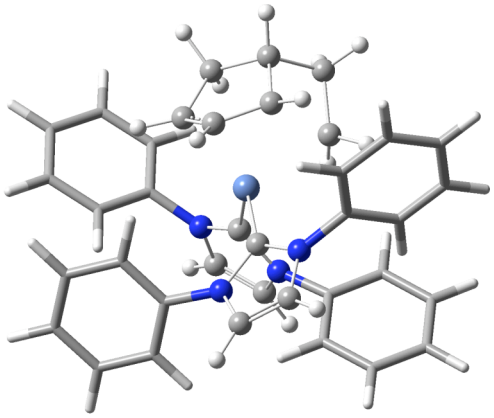
C	4.51568	-0.88715	0.02176
C	4.276	0.3471	-0.9342
C	3.30955	-0.19092	-1.98958
C	3.13487	-1.59224	-1.85758
C	3.95279	-2.14956	-0.68419
H	5.15893	0.80396	-1.40245
H	3.1771	0.34515	-2.93123
H	2.84526	-2.24777	-2.68151
H	4.7674	-2.78922	-1.06242
H	3.35558	-2.76891	0.00277
H	5.5539	-1.01833	0.34813
C	3.63545	-0.17809	1.11216
H	2.62391	-0.59898	1.16143
H	4.05674	-0.13468	2.12301
C	2.92335	0.97607	0.29039
H	3.55527	1.86932	0.37943
H	1.91264	1.13874	0.6801
C	0.09084	-0.23657	0.19921
C	-1.60933	0.64824	1.50176
C	-1.59376	-0.70531	1.71958
H	-2.24509	1.41486	1.91526
H	-2.2152	-1.31767	2.35338
N	-0.56056	-1.23	0.92591
N	-0.58701	0.91982	0.57764
C	-0.20083	-2.64842	0.85453
H	0.6479	-2.74402	0.17259
H	0.0875	-3.02642	1.84317
H	-1.03828	-3.24354	0.46982
C	-0.25941	2.25261	0.06469
H	0.52112	2.14077	-0.69223
H	-1.14024	2.71623	-0.396
H	0.11195	2.90122	0.8679
Ni	1.55161	-0.41614	-0.99827
C	0.68963	-0.62933	-2.7006
C	-0.10582	-1.55104	-4.59308
C	-0.23377	-0.19099	-4.69706
H	-0.54911	-2.32263	-5.38316
H	-0.59471	0.26239	-5.56064
N	0.33288	0.4195	-3.66977
N	0.31771	-1.87538	-3.36865
C	0.42253	-3.09742	-2.55837
H	-0.1531	-3.86239	-3.03625
H	1.26382	-3.53899	-2.0663
H	-0.18576	-2.59029	-1.83886
C	0.7974	1.77038	-3.36819
H	-0.03301	2.39598	-3.62104
H	0.80751	1.60074	-2.31177
H	1.70775	2.25036	-3.66108



A1-dimer
(oniom(rb3lyp/lanl2dz:rhf/lanl2dz)) with benzene groups (low level) to model IPr ligands.

E= -888.3537219
ZPE= 0.649650
$\mathbf{H}_{corr}$= 0.684998
$\mathbf{G}_{corr}$= 0.578522
$\mathbf{E}_{tot}$= -1811.570516
$\mathbf{H}_{tot}$= -1811.535168
$\mathbf{G}_{tot}$= -1811.641644

C	0	0.08096	-3.77465	-0.69131	H
C	0	0.79579	-2.53355	-1.26869	H
C	0	-0.17502	-1.76002	-2.03265	H
C	0	-1.43873	-1.98328	-1.4155	H
C	0	-1.42185	-3.32617	-0.66137	H
H	0	1.83251	-2.61511	-1.58159	H
H	0	0.04313	-1.14502	-2.89807	H
H	0	-2.37136	-1.57028	-1.79102	H
H	0	-2.06952	-4.07262	-1.1521	H
H	0	-1.77265	-3.23662	0.37352	H
H	0	0.19571	-4.66712	-1.32998	H
C	0	0.75492	-3.85818	0.68652	H
H	0	0.08387	-4.21404	1.48219	H
H	0	1.62808	-4.52935	0.67252	H
C	0	1.1797	-2.37388	0.84276	H
H	0	2.25914	-2.211	0.8349	H
H	0	0.73004	-1.8748	1.70137	H
C	0	-1.01233	-0.02832	1.2356	H
C	0	-1.36991	0.92896	3.35603	H
C	0	-2.57179	0.45956	2.92554	H
H	0	-1.09388	1.44083	4.26363	H
H	0	-3.54651	0.48478	3.38477	H
N	0	-2.3577	-0.11709	1.65576	H
N	0	-0.43235	0.63694	2.34231	H
Ni	0	-0.05136	-0.68725	-0.29882	H
C	0	1.05519	0.80451	-1.03478	H
C	0	1.58812	2.92401	-1.90592	H
C	0	2.74952	2.21477	-1.84634	H
H	0	1.38872	3.92188	-2.26193	H
H	0	3.7569	2.48456	-2.11957	H
N	0	2.42349	0.94153	-1.33371	H
N	0	0.56864	2.07033	-1.42687	H
C	0	3.45197	-0.07976	-1.22824	L H
31	0.	0.			
C	0	3.82114	-0.78071	-2.37426	L
C	0	4.11173	-0.29064	-0.02414	L
C	0	4.85785	-1.70982	-2.31051	L
H	0	3.29415	-0.61214	-3.29213	L
C	0	5.14775	-1.22259	0.03756	L
H	0	3.81148	0.25186	0.84629	L
C	0	5.52302	-1.93207	-1.10321	L
H	0	5.13651	-2.25798	-3.18861	L
H	0	5.65032	-1.39623	0.96846	L
H	0	6.31728	-2.65056	-1.05234	L
C	0	-0.82167	2.46243	-1.54977	L H
32	0.	0.			
C	0	-1.28076	3.58963	-0.87013	L
C	0	-1.65471	1.78869	-2.44004	L
C	0	-2.57765	4.05283	-1.08989	L
H	0	-0.63323	4.1038	-0.18802	L
C	0	-2.94883	2.2575	-2.66008	L
H	0	-1.29577	0.92027	-2.94999	L
C	0	-3.41226	3.39186	-1.99219	L
H	0	-2.92838	4.92088	-0.56743	L
H	0	-3.58554	1.74076	-3.35039	L
H	0	-4.40544	3.75433	-2.17063	L
C	0	-3.4963	-0.69614	0.95946	L H
23	0.	0.			
C	0	-3.96853	-1.94442	1.35088	L
C	0	-4.16918	0.04792	-0.00167	L
C	0	-5.1155	-2.46533	0.75351	L
H	0	-3.43802	-2.50437	2.09408	L
C	0	-5.31454	-0.47508	-0.59904	L
H	0	-3.79635	1.01018	-0.27931	L
C	0	-5.78906	-1.73309	-0.22429	L
H	0	-5.47186	-3.43413	1.04268	L
H	0	-5.83015	0.09253	-1.34875	L
H	0	-6.66818	-2.13641	-0.68731	L
C	0	0.94848	1.04968	2.53292	L H
24	0.	0.			
C	0	1.79586	0.26539	3.31241	L
C	0	1.36854	2.29301	2.06836	L
C	0	3.07199	0.73133	3.62774	L
H	0	1.46293	-0.68974	3.66161	L
C	0	2.64777	2.75363	2.37774	L
H	0	0.70048	2.89053	1.48475	L
C	0	3.49962	1.97648	3.16416	L
H	0	3.72175	0.12844	4.23067	L
H	0	2.97027	3.71023	2.01705	L
H	0	4.47905	2.33557	3.41229	L



TS-A1-dimer
(oniom(rb3lyp/lanl2dz:rhf/lanl2dz)) with benzene groups (low level) to model IPr ligands. Note: the oxidation barrier only only slightly (from 41.2 to 42.1 kcal/mol) when ligands were model using benzene vs methyl groups. We suspect model of ligand to not have much effect on barriers as was noted in previously.[5]

E= -888.2826067
ZPE= 0.646951
$\mathbf{H}_{corr}$= 0.682277
$\mathbf{G}_{corr}$= 0.576105
$\mathbf{E}_{tot}$= -1811.503373
$\mathbf{H}_{tot}$= -1811.468047
$\mathbf{G}_{tot}$= -1811.574219

C	0	-0.17983	3.7486	-0.13303	H
C	0	-0.90453	2.63771	-0.93625	H
C	0	0.05263	1.97597	-1.80653	H
C	0	1.34252	2.14435	-1.21297	H
C	0	1.34161	3.39112	-0.30473	H
H	0	-1.93085	2.80131	-1.26241	H
H	0	-0.17339	1.49256	-2.74979	H
H	0	2.25259	1.85715	-1.74078	H
H	0	1.8879	4.22804	-0.77393	H
H	0	1.81307	3.21604	0.67301	H
H	0	-0.37538	4.75447	-0.53757	H
C	0	-0.77103	3.50342	1.27133	H
H	0	-0.00342	3.49949	2.05652	H
H	0	-1.52144	4.25896	1.55363	H
C	0	-1.39389	2.09994	1.05004	H
H	0	-2.48473	2.12907	0.92081	H
H	0	-1.15093	1.37416	1.82834	H
C	0	0.92352	-0.12809	1.2577	H
C	0	1.22503	-1.40335	3.19064	H
C	0	2.45028	-0.90418	2.84219	H
H	0	0.93437	-2.03195	4.01754	H
H	0	3.41367	-1.02187	3.31252	H
N	0	2.26145	-0.14067	1.67892	H
N	0	0.31175	-0.93683	2.23164	H
Ni	0	0.02407	0.69532	-0.23712	H
C	0	-0.92428	-0.80195	-1.18522	H
C	0	-1.2	-2.75831	-2.42619	H
C	0	-2.42476	-2.14792	-2.36257	H
H	0	-0.90115	-3.67621	-2.90745	H
H	0	-3.3754	-2.44164	-2.77915	H
N	0	-2.24731	-0.97382	-1.61002	H
N	0	-0.30544	-1.94096	-1.71504	H
C	0	-3.32276	-0.01438	-1.32055	L H
31	0.	0.			
C	0	-3.61568	1.00084	-2.23158	L
C	0	-4.05043	-0.11899	-0.13518	L
C	0	-4.63563	1.91161	-1.95692	L
H	0	-3.0413	1.08351	-3.16566	L
C	0	-5.07137	0.79138	0.13926	L
H	0	-3.81981	-0.9192	0.58289	L
C	0	-5.36397	1.80667	-0.77129	L
H	0	-4.86616	2.71223	-2.67467	L
H	0	-5.64521	0.7084	1.07376	L
H	0	-6.16815	2.52486	-0.55497	L
C	0	1.13033	-2.22422	-1.57631	L H
32	0.	0.			
C	0	1.57245	-3.13104	-0.61262	L
C	0	2.05065	-1.58655	-2.40813	L
C	0	2.93467	-3.39955	-0.48041	L
H	0	0.8467	-3.63302	0.04353	L
C	0	3.41324	-1.85578	-2.27667	L
H	0	1.70234	-0.87195	-3.16784	L
C	0	3.85537	-2.76201	-1.31292	L
H	0	3.28329	-4.11382	0.27957	L
H	0	4.13861	-1.35316	-2.93294	L
H	0	4.92938	-2.97392	-1.20853	L
C	0	3.36199	0.55816	0.99968	L H
23	0.	0.			
C	0	3.63942	1.88984	1.30972	L
C	0	4.12894	-0.11006	0.04531	L
C	0	4.68317	2.55328	0.665	L
H	0	3.03409	2.4166	2.06161	L
C	0	5.17367	0.55314	-0.59898	L
H	0	3.91053	-1.15969	-0.19904	L
C	0	5.4508	1.88465	-0.28941	L
H	0	4.90151	3.60311	0.90887	L
H	0	5.77848	0.0259	-1.35111	L
H	0	6.27375	2.40793	-0.79757	L
C	0	-1.11553	-1.28783	2.25536	L H
24	0.	0.			
C	0	-2.03616	-0.42525	2.85105	L
C	0	-1.54947	-2.48315	1.68225	L
C	0	-3.39032	-0.7583	2.87419	L
H	0	-1.69363	0.51668	3.30347	L
C	0	-2.90415	-2.81599	1.70444	L
H	0	-0.82403	-3.16304	1.21256	L
C	0	-3.82455	-1.95389	2.30039	L
H	0	-4.11595	-0.07875	3.34425	L
H	0	-3.24606	-3.75832	1.25213	L
H	0	-4.89232	-2.21625	2.3187	L

C	-1.49944	-0.4848	-0.61067
C	-1.20684	0.97274	-0.9834
C	-0.4676	1.51069	0.01836
C	-0.26695	0.41936	1.07514
C	-1.60894	-0.36151	0.94059
H	-1.46823	1.43446	-1.92974
H	-0.00593	2.49124	0.04907
H	0.03304	0.75163	2.07049
H	-2.47078	0.23077	1.26123
H	-1.61113	-1.32939	1.45859
H	-2.32984	-0.96211	-1.13514
C	-0.13211	-1.26003	-0.74345
H	-0.27464	-2.33862	-0.61067
H	0.34333	-1.09326	-1.71374
C	0.71798	-0.66508	0.45011
H	0.90277	-1.44354	1.20198
F	1.98818	-0.13549	0.0615

2-5

E= -371.9310949
ZPE= 0.145855
$\mathbf{H}_{corr}$ = 0.152784
$\mathbf{G}_{corr}$= 0.11592
$\mathbf{E}_{tot}$= -371.78524
$\mathbf{H}_{tot}$= -371.778311
$\mathbf{G}_{tot}$= -371.8151749

C	2.60411	-1.48428	0.01921
C	2.36443	-0.25004	-0.93675
C	1.68461	-0.90783	-2.13778
C	1.2233	-2.18937	-1.86013
C	2.04122	-2.74669	-0.68674
H	3.24736	0.20683	-1.405
H	1.67432	-0.39996	-3.10401
H	0.93369	-2.8449	-2.68406
H	2.85583	-3.38635	-1.06497
H	1.44401	-3.36604	0.00022
H	3.64233	-1.61546	0.34557
C	1.72388	-0.77523	1.10961
H	0.71234	-1.19611	1.15888
H	2.14517	-0.73181	2.12046
C	1.59425	0.79836	0.64761
H	2.30748	1.52587	1.0565
H	0.63426	1.29603	0.47264
Ni	0.22679	-0.20399	-0.80332
C	-1.6055	-0.05712	-0.333