Nickel Catalyzed Alkyl Coupling Reactions: Evaluation of Computational Methods
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Supporting Information

Table of Contents
M06 optimized geometries and M06, MP2, CCSD, and CCSD(T) energies

Table S1 Ni complex Anti-**1**	S2
Table S2 Ni complex Syn-**1**	S2
Table S3 Ni complex **2**	S3
Table S4 Ni complex Anti-**3**	S4
Table S5 Ni complex Syn-**3**	S5
Table S6 Ni complex Me anion Anti-**4**	S5
Table S7 Ni complex Me anion Syn-**4**	S6
Table S8 Ni complex Me anion **5**	S7
Table S9 Ni complex Me anion Anti-**6**	S8
Table S10 Ni complex Me anion Syn-**6**	S9
Table S11 Ni complex Me anion Anti-**7**	S10
Table S12 Ni complex Me anion Syn-**7**	S10
Table S13 S_N2 TS **8**	S11
Table S14 S_N2 TS **9**	S12
Table S15 S_N2 TS **10**	S13
Table S16 S_N2 TS **11**	S14
Table S17 S_N2 TS **12**	S15
Table S18 S_N2 TS **13**	S16
Table S19 S_N2 TS **14**	S17
Table S20 S_N2 TS **15**	S18
Table S21 S_N2 TS **16**	S19
Table S22 S_N2 TS **17**	S20
Table S23 S_N2 TS **18**	S21
Table S24 S_N2 TS **19**	S22
Table S25 Ni dimethyl complex Anti-**20**	S23
Table S26 Ni dimethyl complex Syn-**20**	S24
Table S27 Ni dimethyl complex **21**	S24
Table S28 Ni dimethyl complex Anti-**22**	S25
Table S29 Ni dimethyl complex Syn-**22**	S26
Table S30 Ni dimethyl complex Anti-**23**	S27
Table S31 Ni dimethyl complex Syn-**23**	S28
Table S32 Reductive elimination TS **24**	S29
Table S33 Reductive elimination TS **25**	S30
Table S34 Reductive elimination TS **26**	S31
Table S35 Reductive elimination TS **27**	S32
Table S36 Reductive elimination TS **28**	S33
Table S37 Reductive elimination TS **29**	S34
Table S38 Reductive elimination TS **30**	S35
Sample input file for CCSD(T)/aug-cc-pvdz calculation with Ni.	

Table S1 Ni complex Anti-**1**

SCF Done: E(RM06) = -1742.56172135 A.U. after 10 cycles
EUMP2 = -0.17406908739706D+04
E(CCSD)= -1740.7488588
CCSD(T)= -0.17408124690D+04

Framework group C1[X(C6H10Ni)]
Deg. of freedom 45
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000041	-0.000097	-0.000722
2	6	0	1.576726	-1.220850	0.230779
3	6	0	1.942182	0.000112	-0.368906
4	6	0	1.576504	1.220917	0.230941
5	1	0	1.695169	-2.152548	-0.319409
6	1	0	2.201295	0.000212	-1.431663
7	1	0	1.694734	2.152719	-0.319115
8	6	0	-1.577062	-1.220746	-0.230136
9	6	0	-1.941594	0.000112	0.370307
10	6	0	-1.576840	1.220812	-0.230298
11	1	0	-1.694512	-2.152636	0.319930
12	1	0	-2.199005	0.000212	1.433475
13	1	0	-1.694078	2.152807	0.319636
14	1	0	1.581780	-1.319551	1.320467
15	1	0	1.581483	1.319460	1.320644
16	1	0	-1.583907	-1.319082	-1.319853
17	1	0	-1.583610	1.318990	-1.320030

Table S2 Ni complex Syn-**1**

SCF Done: E(RM06) = -1742.56025341 A.U. after 17 cycles
EUMP2 = -0.17406921106373D+04
E(CCSD)= -1740.7487616
CCSD(T)= -0.17408123967D+04

Framework group C1[X(C6H10Ni)]
Deg. of freedom 45
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000023	-0.000163	-0.047801

2	6	0	-1.571849	1.221137	0.208537
3	6	0	-1.945806	0.000194	-0.384691
4	6	0	-1.572180	-1.221052	0.208213
5	1	0	-1.702808	2.153457	-0.337404
6	1	0	-2.216935	0.000382	-1.444341
7	1	0	-1.703466	-2.153145	-0.338042
8	6	0	1.572149	-1.220992	0.208520
9	6	0	1.945799	0.000101	-0.384690
10	6	0	1.571788	1.221207	0.208232
11	1	0	1.703483	-2.153259	-0.337426
12	1	0	2.216959	-0.000024	-1.444331
13	1	0	1.702717	2.153377	-0.337980
14	1	0	1.558495	-1.318241	1.298469
15	1	0	1.558192	1.318726	1.298155
16	1	0	-1.558063	1.318337	1.298486
17	1	0	-1.558625	-1.318626	1.298130

Ni complex **2**
SCF Done: E(RM06) = -1856.69262301 A.U. after 13 cycles
EUMP2 = -0.18545440845116D+04
E(CCSD)= -1854.6384022
CCSD(T)= -0.18547245054D+04

Framework group C1[X(C9H10Ni)]
Deg. of freedom 54
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.545338	0.387444	0.042154
2	6	0	0.608217	1.042517	-0.948076
3	6	0	-0.608252	1.042504	0.948075
4	6	0	0.563966	0.011825	1.087474
5	1	0	0.907323	-0.262252	2.092647
6	6	0	-0.000032	2.097965	-0.000003
7	1	0	-0.770963	2.729526	-0.462134
8	1	0	0.770881	2.729550	0.462125
9	6	0	-0.563973	0.011805	-1.087470
10	1	0	-0.907323	-0.262286	-2.092642
11	6	0	-1.545356	0.387405	-0.042154
12	1	0	1.055729	1.392697	-1.884227
13	1	0	-1.055774	1.392676	1.884224
14	6	0	-2.873549	0.229272	0.026064
15	1	0	-3.432023	-0.251990	-0.776705

16	1	0	-3.437584	0.553873	0.899680
17	6	0	2.873534	0.229335	-0.026065
18	1	0	3.437562	0.553943	-0.899684
19	1	0	3.432019	-0.251911	0.776706
20	28	0	0.000028	-1.463009	0.000001

Table S4 Ni complex Anti-**3**

SCF Done: E(RM06) = -1819.91416256 A.U. after 12 cycles
EUMP2 = -0.18178411597636D+04
E(CCSD)= -1817.9138947
CCSD(T)= -0.18179911822D+04

Framework group C1[X(C8H12Ni)]
Deg. of freedom 57
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.642056	0.000005	-0.000011
2	6	0	-0.820381	1.266644	-0.413444
3	6	0	-2.142492	0.757469	0.127565
4	1	0	-0.725523	1.244798	-1.508649
5	6	0	-2.142478	-0.757503	-0.127564
6	1	0	-2.192405	0.944707	1.212576
7	1	0	-3.013563	1.257127	-0.325482
8	6	0	-0.820359	-1.266651	0.413450
9	1	0	-3.013541	-1.257177	0.325482
10	1	0	-2.192384	-0.944742	-1.212574
11	1	0	-0.725499	-1.244782	1.508654
12	6	0	0.209736	1.884600	0.320832
13	6	0	1.552634	1.793798	-0.147707
14	1	0	0.030694	2.106326	1.378858
15	1	0	2.362322	2.135431	0.494591
16	1	0	1.752340	1.881006	-1.219802
17	6	0	0.209767	-1.884606	-0.320815
18	6	0	1.552662	-1.793773	0.147721
19	1	0	0.030727	-2.106359	-1.378836
20	1	0	2.362359	-2.135413	-0.494562
21	1	0	1.752364	-1.880939	1.219821

Table S5 Ni complex Syn-**3**
SCF Done: E(RM06) = -1819.90734165 A.U. after 13 cycles
EUMP2 = -0.18178414866098D+04
E(CCSD)= -1817.9079055
CCSD(T)= -0.18179848698D+04

Framework group C1[X(C8H12Ni)]
Deg. of freedom 57
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.613532	0.172873	-0.054933
2	6	0	1.127904	1.021032	-0.445158
3	6	0	2.306811	0.136496	-0.052759
4	1	0	0.996421	1.198878	-1.520404
5	6	0	1.791524	-1.283964	0.279667
6	1	0	3.022363	0.103063	-0.886673
7	1	0	2.858427	0.557486	0.802124
8	6	0	0.428700	-1.468079	-0.367690
9	1	0	2.515893	-2.060773	-0.014147
10	1	0	1.665385	-1.374964	1.369933
11	1	0	0.399196	-1.555576	-1.460709
12	6	0	0.353393	1.805902	0.432341
13	6	0	-0.975906	2.157187	0.068363
14	1	0	0.635443	1.835221	1.491466
15	1	0	-1.620290	2.639439	0.800828
16	1	0	-1.194986	2.413669	-0.973210
17	6	0	-0.747039	-1.735454	0.369217
18	6	0	-2.010091	-1.295231	-0.099204
19	1	0	-0.640811	-1.929266	1.442832
20	1	0	-2.879899	-1.377621	0.549247
21	1	0	-2.230013	-1.317323	-1.171838

Table S6 Ni complex Me anion Anti-**4**
SCF Done: E(RM06) = -1782.44196409 A.U. after 12 cycles
EUMP2 = -0.17804105986980D+04
E(CCSD)= -1780.5054037
CCSD(T)= -0.17805749264D+04

Framework group C1[X(C7H13Ni)]
Deg. of freedom 57
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.447354	0.238966	0.139958
2	6	0	-1.373510	0.537585	0.881975
3	6	0	-2.203963	0.315710	-0.295370
4	6	0	-2.950084	-0.770963	-0.604095
5	1	0	-1.408372	1.576862	1.240585
6	1	0	-2.172041	1.119566	-1.043315
7	1	0	-3.465697	-0.864410	-1.560904
8	6	0	0.553961	-1.747226	0.653585
9	6	0	1.297026	-1.432583	-0.495224
10	6	0	2.271806	-0.411397	-0.470223
11	1	0	-0.325905	-2.387610	0.575126
12	1	0	0.899084	-1.750604	-1.465847
13	1	0	2.711663	-0.056585	-1.403523
14	1	0	-1.605339	-0.164570	1.698596
15	1	0	-3.025145	-1.618647	0.082909
16	1	0	1.008647	-1.678358	1.646914
17	1	0	2.886744	-0.259341	0.422937
18	6	0	0.699677	2.139644	-0.223425
19	1	0	0.877499	2.640611	0.746874
20	1	0	1.542538	2.386737	-0.890870
21	1	0	-0.219062	2.580676	-0.651653

Table S7 Ni complex Me anion Syn-**4**

SCF Done: E(RM06) = -1782.42244403 A.U. after 15 cycles

EUMP2 = -0.17803809691822D+04

E(CCSD)= -1780.4911971

CCSD(T)= -0.17805692286D+04

Framework group C1[X(C7H13Ni)]

Deg. of freedom 57

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000009	0.125787	-0.021037
2	6	0	1.589038	-0.153667	1.220045
3	6	0	1.610343	-1.035599	0.108944
4	6	0	1.578546	-0.431747	-1.175882
5	1	0	1.431672	-0.555740	2.224525
6	1	0	1.381822	-2.098032	0.234177
7	1	0	1.413790	-1.056162	-2.058215

8	6	0	-1.578612	-0.431607	-1.175832
9	6	0	-1.610343	-1.035614	0.108923
10	6	0	-1.589001	-0.153789	1.220098
11	1	0	-1.413934	-1.055884	-2.058275
12	1	0	-1.381808	-2.098057	0.234034
13	1	0	-1.431611	-0.555920	2.224552
14	1	0	-2.148357	0.483830	-1.358711
15	1	0	-2.149450	0.784852	1.180299
16	1	0	2.149497	0.784963	1.180170
17	1	0	2.148293	0.483651	-1.358949
18	6	0	-0.000003	2.176646	-0.180124
19	1	0	-0.000531	2.642907	0.823879
20	1	0	0.892430	2.554927	-0.717269
21	1	0	-0.891875	2.554901	-0.718211

Table S8 Ni complex Me anion **5**

SCF Done: E(RM06) = -1896.63273430 A.U. after 20 cycles

EUMP2 = -0.18943501004165D+04

E(CCSD)= -1894.4491720

CCSD(T)= -0.18945387397D+04

Framework group C1[X(C10H13Ni)]

Deg. of freedom 66

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685596	-1.499008	-0.061854
2	6	0	-1.067121	-0.584480	1.096893
3	6	0	-1.606309	0.628214	-0.705152
4	6	0	-0.702959	-0.555077	-1.164435
5	1	0	-0.749011	-0.890231	-2.205644
6	6	0	-2.349825	0.029639	0.502872
7	1	0	-2.817403	0.796198	1.142614
8	1	0	-3.089302	-0.739623	0.228951
9	6	0	-0.043809	0.590601	0.983327
10	1	0	0.435139	0.971936	1.891834
11	6	0	-0.657244	1.543934	0.038469
12	1	0	-1.135437	-1.072573	2.077824
13	1	0	-2.214507	1.108583	-1.483809
14	6	0	-0.468765	2.865831	-0.132375
15	1	0	0.272258	3.413847	0.453139
16	1	0	-0.987660	3.413901	-0.921046
17	6	0	-0.386920	-2.822773	0.042834

18	1	0	-0.334959	-3.309035	1.018005
19	1	0	-0.094954	-3.413895	-0.827420
20	28	0	1.132979	-0.149141	-0.334644
21	6	0	2.856329	0.270982	0.438877
22	1	0	3.033683	-0.224038	1.409204
23	1	0	3.671561	-0.046615	-0.243596
24	1	0	2.960492	1.360317	0.593249

Table S9 Ni complex Me anion Anti-**6**

SCF Done: E(RM06) = -1859.80219581 A.U. after 17 cycles
EUMP2 = -0.18575703195116D+04
E(CORR)= -1857.6801862
CCSD(T)= -0.18577634601D+04

Framework group C1[X(C9H15Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.539392	-0.554357	0.046630
2	6	0	-1.229948	0.181033	0.611300
3	6	0	-0.837942	1.595280	1.067442
4	1	0	-1.614715	-0.420045	1.452579
5	6	0	-0.031340	2.315454	-0.024734
6	1	0	-1.704641	2.214757	1.391231
7	1	0	-0.190310	1.494735	1.955492
8	6	0	0.862723	1.303032	-0.707724
9	1	0	-0.714037	2.757432	-0.768032
10	1	0	0.532746	3.164536	0.404025
11	1	0	0.697845	1.122888	-1.777202
12	6	0	-2.138856	0.112707	-0.526931
13	6	0	-3.167649	-0.743516	-0.712955
14	1	0	-1.938563	0.821421	-1.343407
15	1	0	-3.732101	-0.773073	-1.646024
16	1	0	-3.425666	-1.486299	0.045959
17	6	0	2.002816	0.742989	-0.110609
18	6	0	2.495802	-0.519130	-0.542284
19	1	0	2.312258	1.119670	0.874339
20	1	0	3.298802	-1.000706	0.018146
21	1	0	2.452801	-0.780978	-1.605059
22	6	0	0.166544	-2.394365	0.556891
23	1	0	0.071515	-2.451915	1.657268
24	1	0	-0.807888	-2.689448	0.126478

25	1	0	0.926092	-3.131887	0.246204

Table S10 Ni complex Me anion Syn-**6**

SCF Done: E(RM06) = -1859.80369521 A.U. after 13 cycles

EUMP2 = -0.18575726674977D+04

E(CCSD)= -1857.6819448

CCSD(T)= -0.18577650990D+04

Framework group C1[X(C9H15Ni)]

Deg. of freedom 69

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.491259	-0.533031	-0.199725
2	6	0	-1.245805	0.398341	-0.580226
3	6	0	-0.945893	1.899972	-0.746797
4	1	0	-1.733475	-0.019371	-1.476463
5	6	0	0.200529	2.315322	0.180001
6	1	0	-0.609525	2.073639	-1.784220
7	1	0	-1.838555	2.547370	-0.600198
8	6	0	1.297432	1.318929	-0.069775
9	1	0	0.501909	3.365205	0.001229
10	1	0	-0.120675	2.256393	1.234449
11	1	0	1.760923	1.365752	-1.065403
12	6	0	-2.021715	0.087221	0.619270
13	6	0	-3.048847	-0.779854	0.748607
14	1	0	-1.713496	0.619665	1.531998
15	1	0	-3.502995	-0.994843	1.716976
16	1	0	-3.410738	-1.355742	-0.106539
17	6	0	1.831672	0.430048	0.872318
18	6	0	2.411305	-0.796995	0.442137
19	1	0	1.508846	0.525855	1.917260
20	1	0	2.686112	-1.546572	1.186141
21	1	0	3.006066	-0.820412	-0.477173
22	6	0	-0.088355	-2.356470	-0.569910
23	1	0	-1.019052	-2.386286	-1.163649
24	1	0	0.682611	-2.951926	-1.090751
25	1	0	-0.295161	-2.852931	0.394884

Table S11 Ni complex Me anion Anti-**7**
SCF Done: E(RM06) = -1859.79744969 A.U. after 15 cycles
EUMP2 = -0.18575622303082D+04
E(CCSD)= -1857.6707609
CCSD(T)= -0.18577551003D+04

Framework group C1[X(C9H15Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.971525	-0.092594	-0.007332
2	6	0	2.214712	-1.237867	-0.355202
3	6	0	2.974875	-0.040177	0.108562
4	1	0	2.130612	-1.357969	-1.445854
5	6	0	2.152879	1.247712	-0.190681
6	1	0	3.139612	-0.093266	1.201166
7	1	0	3.970256	0.069622	-0.356950
8	6	0	0.770266	1.298375	0.391391
9	1	0	2.744707	2.113290	0.164288
10	1	0	2.073945	1.356394	-1.287765
11	1	0	0.696146	1.236631	1.485270
12	6	0	1.128143	-1.581666	0.396731
13	6	0	-0.192289	-1.949174	-0.039769
14	1	0	1.213314	-1.375835	1.475422
15	1	0	-0.780555	-2.588278	0.632618
16	1	0	-0.266808	-2.281555	-1.087052
17	6	0	-0.321435	1.801344	-0.313639
18	6	0	-1.649400	1.785785	0.173073
19	1	0	-0.166739	2.009787	-1.380605
20	1	0	-2.459956	2.122136	-0.474974
21	1	0	-1.840585	1.891180	1.246390
22	6	0	-2.740489	-0.879998	-0.112575
23	1	0	-2.746903	-1.762321	-0.774578
24	1	0	-2.997555	-1.226869	0.905249
25	1	0	-3.530348	-0.186322	-0.444695

Table S12 Ni complex Me anion Syn-**7**
SCF Done: E(RM06) = -1859.81505436 A.U. after 17 cycles
EUMP2 = -0.18575868386025D+04
E(CORR)= -1857.6914447
CCSD(T)= -0.18577740938D+04

Framework group C1[X(C9H15Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.926547	-0.116909	-0.077258
2	6	0	-2.321086	-0.989772	0.623658
3	6	0	-2.723773	0.112181	-0.299493
4	1	0	-2.889992	-1.100132	1.551823
5	6	0	-1.938940	1.425257	-0.048978
6	1	0	-2.574208	-0.180126	-1.354397
7	1	0	-3.799628	0.332338	-0.190027
8	6	0	-0.489513	1.410568	-0.437199
9	1	0	-2.463084	2.238560	-0.585971
10	1	0	-2.022588	1.664346	1.026268
11	1	0	-0.280092	1.494142	-1.512530
12	6	0	-1.186892	-1.715078	0.448245
13	6	0	-0.238175	-1.618998	-0.649893
14	1	0	-0.917843	-2.413972	1.251119
15	1	0	0.354990	-2.531957	-0.795283
16	1	0	-0.687602	-1.296747	-1.602945
17	6	0	0.522853	1.758214	0.470933
18	6	0	1.897767	1.626025	0.176666
19	1	0	0.224164	1.860864	1.522720
20	1	0	2.632437	1.755528	0.973332
21	1	0	2.269614	1.828717	-0.833072
22	6	0	2.467072	-1.291605	0.102392
23	1	0	2.198065	-2.107218	0.799366
24	1	0	2.685557	-1.758049	-0.875415
25	1	0	3.391008	-0.813597	0.470243

Table S13 S_N2 TS **8**
SCF Done: E(RM06) = -2282.47055095 A.U. after 16 cycles
EUMP2 = -0.22797579637661D+04
E(CCSD)= -2279.8718985
CCSD(T)= -0.22799611343D+04

Framework group C1[X(C8H16ClNi)]
Deg. of freedom 72
Standard orientation:

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

1	28	0	1.010557	-0.155788	0.260947
2	6	0	0.459144	1.599472	0.980637
3	1	0	-0.215303	1.449119	1.835094
4	6	0	1.410187	0.394946	-1.734625
5	1	0	0.449913	0.144957	-2.192666
6	6	0	-0.084093	2.552803	0.011789
7	6	0	-1.382487	2.859032	-0.167348
8	1	0	0.642111	3.016522	-0.666574
9	1	0	-1.709675	3.533750	-0.958129
10	1	0	-2.164694	2.413947	0.452015
11	6	0	2.267207	-0.610225	-1.268500
12	6	0	1.788444	-1.811174	-0.720187
13	1	0	3.295209	-0.318869	-1.023021
14	1	0	2.474651	-2.481202	-0.202191
15	1	0	0.889849	-2.281908	-1.125015
16	6	0	0.950490	-1.063962	1.975590
17	1	0	2.002706	-1.096654	2.312457
18	1	0	0.356743	-0.519915	2.725369
19	1	0	0.582420	-2.098880	1.909853
20	6	0	-1.174865	-0.577339	0.168513
21	1	0	-1.287220	0.221675	-0.556672
22	1	0	-1.490395	-0.404865	1.188224
23	1	0	-0.979309	-1.595900	-0.139375
24	17	0	-3.518918	-1.114467	-0.334611
25	1	0	1.456237	1.897509	1.354430
26	1	0	1.818620	1.367387	-2.007127

Table S14 S_N2 TS **9**

SCF Done: E(RM06) = -2282.47431830 A.U. after 12 cycles
EUMP2 = -0.22797642056122D+04
E(CCSD)= -2279.8772585
CCSD(T)= -0.22799671617D+04

Framework group C1[X(C8H16ClNi)]
Deg. of freedom 72
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.497576	0.327364	0.176770
2	6	0	1.039852	-1.363207	-0.693364
3	1	0	0.749291	-2.213367	-0.060302
4	6	0	0.812526	1.556809	-1.476790

5	1	0	1.902165	1.630069	-1.407113
6	6	0	2.492040	-1.233290	-0.823436
7	6	0	3.430097	-1.720551	0.012896
8	1	0	2.842743	-0.635451	-1.674305
9	1	0	4.492296	-1.525708	-0.135312
10	1	0	3.150553	-2.311591	0.887889
11	6	0	0.007647	2.185933	-0.516606
12	6	0	0.407075	2.275082	0.826506
13	1	0	-1.056948	2.308477	-0.741258
14	1	0	-0.300910	2.599087	1.589367
15	1	0	1.464424	2.398169	1.081211
16	6	0	0.548150	-0.400800	1.978262
17	1	0	-0.138612	0.099703	2.677945
18	1	0	0.354197	-1.484015	2.006691
19	1	0	1.583589	-0.223411	2.318823
20	6	0	-1.639801	-0.380428	0.067291
21	1	0	-1.923655	0.389837	0.771033
22	1	0	-1.491291	-1.390395	0.421268
23	1	0	-1.603268	-0.177212	-0.994566
24	17	0	-3.970130	-0.827111	-0.223682
25	1	0	0.416261	1.340284	-2.469538
26	1	0	0.533722	-1.427072	-1.667365

Table S15 S_N2 TS **10**

SCF Done: E(RM06) = -2282.47015123 A.U. after 17 cycles
EUMP2 = -0.22797282739786D+04
E(CORR)= -2279.8720083
CCSD(T)= -0.22799579437D+04

Framework group C1[X(C8H16ClNi)]
Deg. of freedom 72
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.966111	-0.151303	0.110661
2	6	0	-1.026661	1.634878	-0.779523
3	1	0	-1.837515	2.137980	-0.223499
4	6	0	-1.799866	-1.200934	-1.490543
5	1	0	-2.824284	-0.841118	-1.351117
6	6	0	0.208376	2.420362	-0.751282
7	6	0	0.502310	3.451965	0.060424
8	1	0	0.993198	2.096924	-1.447492
9	1	0	1.478466	3.936591	0.044850

10	1	0	-0.226804	3.828839	0.781891
11	6	0	-1.221078	-2.070765	-0.560089
12	6	0	-1.532168	-1.989979	0.809085
13	1	0	-0.292021	-2.576305	-0.842569
14	1	0	-0.941529	-2.546032	1.537917
15	1	0	-2.545660	-1.728702	1.129697
16	6	0	-0.765819	0.605675	1.882812
17	1	0	-0.223609	1.562224	1.858932
18	1	0	-1.808684	0.791411	2.200726
19	1	0	-0.293624	-0.065690	2.615393
20	6	0	1.239846	-0.400980	0.212576
21	1	0	1.159598	-0.525979	-0.860968
22	1	0	1.201917	-1.258601	0.870103
23	1	0	1.529920	0.560421	0.614858
24	17	0	3.577661	-0.949931	-0.117936
25	1	0	-1.415467	-1.143829	-2.508641
26	1	0	-1.352685	1.455835	-1.814447

Table S16 S_N2 TS **11**

SCF Done: E(RM06) = -2282.47297104 A.U. after 20 cycles
EUMP2 = -0.22797597950890D+04
E(CORR)= -2279.8747973
CCSD(T)= -0.22799642762D+04

Framework group C1[X(C8H16ClNi)]
Deg. of freedom 72
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.519937	0.267021	0.176103
2	6	0	-0.841775	-1.473274	-0.696723
3	1	0	-0.526222	-2.295908	-0.041263
4	6	0	-0.631375	1.463009	-1.552512
5	1	0	0.426850	1.609777	-1.782216
6	6	0	-2.291445	-1.345225	-0.818419
7	6	0	-3.223971	-1.770769	0.059812
8	1	0	-2.648154	-0.787509	-1.693759
9	1	0	-4.285522	-1.572239	-0.086472
10	1	0	-2.939267	-2.312035	0.964512
11	6	0	-1.197320	2.070000	-0.422830
12	6	0	-0.464261	2.245879	0.764445
13	1	0	-2.291307	2.092936	-0.354553
14	1	0	-0.974779	2.552867	1.677127

15	1	0	0.601537	2.484226	0.720283
16	6	0	-0.413324	-0.412222	1.998163
17	1	0	-0.192653	-1.490350	2.038375
18	1	0	0.323061	0.123874	2.616600
19	1	0	-1.414589	-0.240465	2.429289
20	6	0	1.691865	-0.299653	0.044315
21	1	0	1.902627	0.567792	0.653538
22	1	0	1.634760	-0.220346	-1.031270
23	1	0	1.649103	-1.273555	0.509460
24	17	0	4.065446	-0.544267	-0.220174
25	1	0	-1.262991	1.194103	-2.399902
26	1	0	-0.327154	-1.523688	-1.665178

Table S17 S_N2 TS **12**

SCF Done: E(RM06) = -2396.67037094 A.U. after 14 cycles
EUMP2 = -0.23936609190290D+04
E(CCSD)= -2393.8182469
CCSD(T)= -0.23939332193D+04

Framework group C1[X(C11H16ClNi)]
Deg. of freedom 81

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464008	-1.449561	-0.374165
2	6	0	-2.401625	-0.514910	0.363229
3	6	0	-1.647902	0.752389	-1.325600
4	6	0	-0.724635	-0.500770	-1.215969
5	1	0	-0.250879	-0.868088	-2.131066
6	6	0	-3.011161	0.213108	-0.851578
7	1	0	-3.715210	1.016853	-0.584711
8	1	0	-3.485358	-0.483688	-1.560174
9	6	0	-1.437334	0.556876	0.959478
10	1	0	-1.595048	0.886283	1.990358
11	6	0	-1.291601	1.571050	-0.103514
12	1	0	-3.086972	-0.992959	1.073996
13	1	0	-1.618128	1.289384	-2.282190
14	6	0	-0.937457	2.866306	-0.043602
15	1	0	-0.684461	3.340135	0.906557
16	1	0	-0.832058	3.468063	-0.947347
17	6	0	-1.360746	-2.785214	-0.216884
18	1	0	-1.961093	-3.313313	0.524677
19	1	0	-0.631831	-3.370582	-0.779508

20	28	0	0.316238	-0.190496	0.531230
21	6	0	0.829832	-0.050613	2.402520
22	1	0	0.167792	-0.628344	3.064907
23	1	0	1.863298	-0.417024	2.525503
24	1	0	0.794714	1.006353	2.714477
25	6	0	1.833378	0.085852	-0.705343
26	1	0	1.919254	-0.743304	0.050445
27	1	0	1.841314	-0.200992	-1.747150
28	1	0	1.873803	1.143279	-0.453585
29	17	0	4.130927	-0.015602	-0.621826

Table S18 S_N2 TS **13**

SCF Done: E(RM06) = -2359.83092326 A.U. after 15 cycles
EUMP2 = -0.23568821080243D+04
E(CCSD)= -2357.0449871
CCSD(T)= -0.23571453908D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.519928	-0.572484	0.471776
2	6	0	1.079593	1.346628	0.502522
3	6	0	2.454946	1.257519	-0.181115
4	1	0	1.187830	1.619915	1.566180
5	6	0	2.328571	0.593556	-1.555855
6	1	0	2.962593	2.242398	-0.252155
7	1	0	3.110861	0.628199	0.445405
8	6	0	1.366836	-0.567952	-1.428925
9	1	0	1.931043	1.313048	-2.287038
10	1	0	3.318736	0.289569	-1.940444
11	1	0	0.492502	-0.584204	-2.087495
12	6	0	0.114036	2.235272	-0.144213
13	6	0	-0.730754	3.078782	0.474943
14	1	0	0.031313	2.157996	-1.236717
15	1	0	-1.493076	3.635402	-0.068544
16	1	0	-0.716889	3.188217	1.562431
17	6	0	1.666486	-1.725279	-0.695404
18	6	0	0.657845	-2.558998	-0.163721
19	1	0	2.663981	-1.786519	-0.238044
20	1	0	0.933617	-3.365997	0.515170
21	1	0	-0.272874	-2.710587	-0.717148

22	6	0	-0.044816	-0.699086	2.319827
23	1	0	0.933202	-0.783856	2.831306
24	1	0	-0.551707	0.206323	2.687455
25	1	0	-0.649078	-1.583319	2.569629
26	6	0	-1.653150	-0.349604	0.179046
27	1	0	-1.362392	-0.266251	-0.862903
28	1	0	-1.853849	0.557091	0.734690
29	1	0	-1.968922	-1.304757	0.574528
30	17	0	-3.923084	-0.181656	-0.755803

Table S19 S_N2 TS **14**

SCF Done: E(RM06) = -2359.83322512 A.U. after 12 cycles
EUMP2 = -0.23569269835205D+04
E(CCSD)= -2357.0511374
CCSD(T)= -0.23571533218D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.309959	0.219605	-0.661278
2	6	0	-1.126547	-0.899494	0.774513
3	6	0	-0.935660	-0.059656	2.048699
4	1	0	-0.572203	-1.850414	0.839429
5	6	0	-1.409575	1.387701	1.825157
6	1	0	-1.422309	-0.509639	2.938831
7	1	0	0.140182	-0.035170	2.284920
8	6	0	-1.210901	1.730149	0.365677
9	1	0	-2.474264	1.492826	2.085824
10	1	0	-0.866420	2.083060	2.486683
11	1	0	-2.111914	1.771317	-0.260767
12	6	0	-2.520330	-1.149455	0.399458
13	6	0	-3.035201	-2.283817	-0.112613
14	1	0	-3.214207	-0.307112	0.528732
15	1	0	-4.078197	-2.355041	-0.421361
16	1	0	-2.409772	-3.164356	-0.274155
17	6	0	-0.016512	2.167460	-0.217182
18	6	0	0.197849	1.978749	-1.606513
19	1	0	0.851409	2.337883	0.431586
20	1	0	1.180066	2.185795	-2.032865
21	1	0	-0.642568	2.091424	-2.299137
22	6	0	-0.069525	-1.144683	-2.012531

23	1	0	0.762485	-0.995751	-2.715959
24	1	0	-0.026440	-2.167361	-1.606733
25	1	0	-1.025390	-1.032158	-2.558384
26	6	0	1.828509	-0.430292	-0.175396
27	1	0	2.265308	0.037748	-1.044589
28	1	0	1.694016	-1.501591	-0.158417
29	1	0	1.635790	0.146821	0.719238
30	17	0	4.045920	-0.715128	0.696311

Table S20 S_N2 TS **15**

SCF Done: E(RM06) = -2359.83186464 A.U. after 12 cycles

EUMP2 = -0.23569237723308D+04

E(CCSD)= -2357.0494795

CCSD(T)=-2357.1515195

Framework group C1[X(C10H18ClNi)]

Deg. of freedom 84

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.587213	-0.497922	0.582822
2	6	0	-1.240475	1.379724	0.190241
3	6	0	-2.319133	1.312245	-0.918690
4	1	0	-1.670584	1.755361	1.134683
5	6	0	-2.070957	0.106930	-1.824366
6	1	0	-3.303327	1.168478	-0.439474
7	1	0	-2.398050	2.253183	-1.497701
8	6	0	-1.896347	-1.035589	-0.865575
9	1	0	-2.892374	-0.040343	-2.549938
10	1	0	-1.145707	0.246823	-2.408792
11	1	0	-2.747443	-1.202072	-0.188197
12	6	0	-0.094865	2.214026	-0.190485
13	6	0	0.529569	3.136156	0.562473
14	1	0	0.306914	2.044446	-1.200294
15	1	0	1.418515	3.658563	0.209997
16	1	0	0.188956	3.360628	1.576324
17	6	0	-0.842642	-1.951181	-0.802215
18	6	0	-0.530748	-2.552448	0.442817
19	1	0	-0.076294	-1.932074	-1.584731
20	1	0	0.377368	-3.147825	0.542172
21	1	0	-1.340214	-2.821052	1.129169
22	6	0	0.056304	-0.142576	2.375914
23	1	0	0.379317	0.900102	2.515476

24	1	0	-0.878412	-0.305539	2.946824
25	1	0	0.827802	-0.820888	2.767662
26	6	0	1.637371	-0.317396	0.201225
27	1	0	1.266169	-0.237220	-0.814144
28	1	0	1.941258	-1.276329	0.594561
29	1	0	1.873058	0.586791	0.744245
30	17	0	3.820385	-0.185209	-0.872053

Table S21 S_N2 TS **16**

SCF Done: E(RM06) = -2359.83581060 A.U. after 14 cycles
EUMP2 = -0.23569260221834D+04
E(CCSD)= -2357.0525677
CCSD(T)= -0.23571553059D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.338604	0.257317	-0.599348
2	6	0	0.921867	-1.034774	0.807223
3	6	0	0.926351	-0.314879	2.165786
4	1	0	0.301804	-1.945232	0.825776
5	6	0	1.387764	1.134979	1.993207
6	1	0	-0.102860	-0.296943	2.562438
7	1	0	1.532700	-0.847359	2.927115
8	6	0	0.571736	1.697833	0.861826
9	1	0	1.275621	1.703146	2.932662
10	1	0	2.459183	1.170649	1.733699
11	1	0	-0.483366	1.900457	1.080407
12	6	0	2.261083	-1.332054	0.289939
13	6	0	2.663447	-2.458043	-0.330236
14	1	0	3.013822	-0.541159	0.412657
15	1	0	3.671094	-2.565449	-0.731685
16	1	0	1.976081	-3.291159	-0.489945
17	6	0	1.081540	2.108473	-0.374552
18	6	0	0.268286	2.107183	-1.533940
19	1	0	2.170622	2.076025	-0.510083
20	1	0	0.725847	2.274281	-2.508996
21	1	0	-0.783317	2.398143	-1.458331
22	6	0	0.088007	-0.903628	-2.140605
23	1	0	-0.014248	-1.959203	-1.839845
24	1	0	-0.771512	-0.620951	-2.768063

25	1	0	1.007173	-0.803721	-2.742071
26	6	0	-1.797055	-0.336431	-0.095322
27	1	0	-2.079229	0.461727	-0.769423
28	1	0	-1.629801	-0.140664	0.953703
29	1	0	-1.807522	-1.356495	-0.450272
30	17	0	-4.128304	-0.519584	0.456591

Table S22 S_N2 TS **17**

SCF Done: E(RM06) = -2359.82886904 A.U. after 14 cycles
EUMP2 = -0.23569023839781D+04
E(CORR)= -2357.0404806
CCSD(T)= -0.23571456450D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.039521	1.024085	0.027131
2	6	0	-1.553029	-0.908836	-1.503435
3	6	0	-2.797952	-1.426580	-0.894832
4	1	0	-0.738299	-1.617292	-1.693080
5	6	0	-2.704993	-1.743508	0.656206
6	1	0	-3.608785	-0.690380	-1.024781
7	1	0	-3.127360	-2.357773	-1.383074
8	6	0	-2.263098	-0.574693	1.443528
9	1	0	-3.700431	-2.112741	0.952060
10	1	0	-1.995294	-2.576760	0.787793
11	1	0	-2.947563	0.281797	1.506135
12	6	0	-1.329523	0.428585	-1.696790
13	6	0	-0.085845	1.093568	-1.963618
14	1	0	-2.191395	1.084767	-1.505263
15	1	0	-0.142832	2.111662	-2.360490
16	1	0	0.713128	0.497030	-2.420310
17	6	0	-0.947233	-0.379509	1.748138
18	6	0	-0.271852	0.866856	1.990262
19	1	0	-0.299381	-1.264321	1.670520
20	1	0	0.644151	0.837118	2.590727
21	1	0	-0.916113	1.719518	2.253117
22	6	0	1.120061	2.588662	0.201139
23	1	0	1.753725	2.758189	-0.681274
24	1	0	0.389382	3.411867	0.282758
25	1	0	1.740177	2.564976	1.108615

26	6	0	1.896655	-0.207276	0.037094
27	1	0	2.103492	-0.073201	1.089261
28	1	0	1.205605	-0.977415	-0.291099
29	1	0	2.432695	0.387357	-0.687873
30	17	0	3.599963	-1.828376	-0.062326

Table S23 S_N2 TS **18**

SCF Done: E(RM06) = -2359.84714629 A.U. after 13 cycles
EUMP2 = -0.23569073909940D+04
E(CCSD)= -2357.0618109
CCSD(T)= -0.23571611683D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.199467	-0.986512	0.308747
2	6	0	-1.508032	2.325098	0.593398
3	6	0	-2.678902	1.762845	-0.144195
4	1	0	-1.223863	3.354800	0.362399
5	6	0	-2.260683	0.925563	-1.375857
6	1	0	-3.295982	1.121678	0.510545
7	1	0	-3.336886	2.577508	-0.484954
8	6	0	-1.744820	-0.440818	-1.053558
9	1	0	-3.137820	0.839873	-2.042803
10	1	0	-1.494858	1.485291	-1.940263
11	1	0	-2.467855	-1.114409	-0.569311
12	6	0	-0.713311	1.599121	1.408792
13	6	0	-0.858733	0.188410	1.766221
14	1	0	0.180539	2.103390	1.794603
15	1	0	-0.330656	-0.063362	2.695500
16	1	0	-1.912761	-0.129069	1.847275
17	6	0	-0.645073	-1.022192	-1.691748
18	6	0	-0.105185	-2.256265	-1.275922
19	1	0	-0.021687	-0.366772	-2.311845
20	1	0	0.846841	-2.596523	-1.685347
21	1	0	-0.766618	-3.051049	-0.916460
22	6	0	0.816101	-2.141042	1.489621
23	1	0	1.270709	-1.608387	2.337845
24	1	0	0.046396	-2.828815	1.886880
25	1	0	1.591188	-2.737512	0.985234
26	6	0	1.746298	0.071352	0.030178

27	1	0	1.142414	0.822115	-0.468116
28	1	0	2.209173	-0.731024	-0.527091
29	1	0	2.011602	0.209389	1.068723
30	17	0	3.646426	1.427222	-0.568782

Table S24 S_N2 TS **19**

SCF Done: E(RM06) = -2359.84618039 A.U. after 14 cycles
EUMP2 = -0.23569351937175D+04
E(CCSD)= -2357.0611500
CCSD(T)= -0.23571635629D+04

Framework group C1[X(C10H18ClNi)]
Deg. of freedom 84

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.077610	0.724850	-0.119478
2	6	0	2.951105	-0.777062	-1.029588
3	6	0	2.729668	-1.777464	0.052309
4	1	0	3.969608	-0.405266	-1.171952
5	6	0	2.378751	-1.115713	1.411631
6	1	0	1.918809	-2.474364	-0.214770
7	1	0	3.632337	-2.391514	0.201817
8	6	0	1.068083	-0.388135	1.484889
9	1	0	2.405445	-1.902683	2.184427
10	1	0	3.196688	-0.417461	1.658865
11	1	0	0.194832	-0.986581	1.766217
12	6	0	1.936866	-0.219800	-1.735338
13	6	0	0.519571	-0.519305	-1.591100
14	1	0	2.193895	0.578286	-2.441965
15	1	0	-0.074873	-0.274332	-2.480065
16	1	0	0.302534	-1.542080	-1.252492
17	6	0	1.018286	0.997919	1.666729
18	6	0	-0.167070	1.758437	1.618464
19	1	0	1.970630	1.531489	1.547147
20	1	0	-0.100358	2.846848	1.625197
21	1	0	-1.096750	1.349363	2.022956
22	6	0	-0.713874	2.077166	-1.257869
23	1	0	0.174632	2.653062	-1.579492
24	1	0	-1.208451	1.670345	-2.152386
25	1	0	-1.406142	2.762856	-0.746912
26	6	0	-2.028947	-0.176972	-0.178445
27	1	0	-2.485807	0.718882	0.213767

28	1	0	-1.608994	-0.919766	0.486578
29	1	0	-2.088826	-0.383575	-1.236546
30	17	0	-4.130407	-1.286101	0.133229

Table S25 Ni dimethyl complex Anti-**20**

SCF Done: E(RM06) = -1822.23615608 A.U. after 18 cycles
EUMP2 = -0.18200590255313D+04
E(CCSD)= -1820.1962537
CCSD(T)= -0.18202778705D+04

Framework group C1[X(C8H16Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000368	0.151457	-0.001330
2	6	0	-1.744919	0.096917	-1.027556
3	1	0	-2.287350	0.958818	-0.638083
4	6	0	1.213415	-1.582303	-0.778658
5	1	0	0.712763	-2.386932	-0.241397
6	6	0	-1.679370	-1.097328	-0.267846
7	6	0	-1.497347	-1.059189	1.104376
8	1	0	-1.468693	-2.027103	-0.798308
9	1	0	-1.242620	-1.970113	1.647032
10	1	0	-1.889955	-0.239176	1.701923
11	6	0	1.939635	-0.630157	-0.086671
12	6	0	1.580635	-0.249932	1.227857
13	1	0	2.597499	0.030221	-0.653714
14	1	0	2.081133	0.601636	1.686764
15	1	0	1.204961	-0.998407	1.926058
16	6	0	-0.348325	1.715761	1.163193
17	1	0	0.460608	2.450690	1.082163
18	1	0	-1.287691	2.175221	0.829107
19	1	0	-0.439814	1.395159	2.208177
20	6	0	0.530306	1.509031	-1.337568
21	1	0	1.440486	1.994447	-0.962915
22	1	0	-0.246047	2.267660	-1.485322
23	1	0	0.734934	0.994571	-2.286239
24	1	0	1.370442	-1.732251	-1.846076
25	1	0	-1.715142	0.027977	-2.114699

Table S26 Ni dimethyl complex Syn-**20**
SCF Done: E(RM06) = -1822.23809653 A.U. after 10 cycles
EUMP2 = -0.18200609723365D+04
E(CCSD)= -1820.1989030
CCSD(T)= -0.18202805074D+04

Framework group C1[X(C8H16Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000118	0.165134	0.000083
2	6	0	-1.710733	-0.016311	1.069720
3	1	0	-2.324463	0.806041	0.699436
4	6	0	1.465126	-1.140947	1.080241
5	1	0	1.947182	-0.347640	1.647397
6	6	0	-1.571599	-1.195415	0.297371
7	6	0	-1.467559	-1.137336	-1.081410
8	1	0	-1.236093	-2.102937	0.804625
9	1	0	-1.170886	-2.018836	-1.649000
10	1	0	-1.948465	-0.342503	-1.647388
11	6	0	1.569923	-1.197383	-0.298589
12	6	0	1.711364	-0.017246	-1.068906
13	1	0	1.233013	-2.103488	-0.807425
14	1	0	1.642082	-0.085239	-2.153868
15	1	0	2.326382	0.803422	-0.697040
16	6	0	0.431553	1.636228	1.254413
17	1	0	-0.313722	2.437327	1.195368
18	1	0	0.482662	1.263273	2.284233
19	1	0	1.411229	2.027612	0.948678
20	6	0	-0.429075	1.637588	-1.253463
21	1	0	-0.479800	1.265564	-2.283627
22	1	0	0.316623	2.438189	-1.193151
23	1	0	-1.408704	2.029305	-0.947936
24	1	0	1.166668	-2.022647	1.646581
25	1	0	-1.641017	-0.086271	2.154526

Table S27 Ni dimethyl complex **21**
SCF Done: E(RM06) = -1936.45006118 A.U. after 11 cycles
EUMP2 = -0.19340339590021D+04
E(CCSD)= -1934.1632020
CCSD(T)= -0.19342624014D+04

Framework group C1[X(C11H16Ni)]
Deg. of freedom 78
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.615197	0.905701	0.182162
2	6	0	-2.028812	-0.312050	-0.623710
3	6	0	-0.745809	-1.178333	1.001770
4	6	0	-0.510658	0.362604	0.989972
5	1	0	-0.179032	0.888191	1.889375
6	6	0	-2.204430	-1.304196	0.542451
7	1	0	-2.443331	-2.326834	0.218139
8	1	0	-2.937853	-0.960163	1.283750
9	6	0	-0.732433	-0.818822	-1.261151
10	1	0	-0.531597	-0.798190	-2.331030
11	6	0	-0.019695	-1.558689	-0.296558
12	1	0	-2.877800	-0.166358	-1.298667
13	1	0	-0.416179	-1.705294	1.902522
14	6	0	1.323197	-1.938905	-0.332658
15	1	0	1.811834	-2.131621	-1.289984
16	1	0	1.779233	-2.402897	0.540171
17	6	0	-2.143710	2.132753	0.174695
18	1	0	-2.983082	2.383225	-0.472764
19	1	0	-1.743829	2.928997	0.801796
20	28	0	1.029208	0.138449	-0.219328
21	6	0	1.021423	2.019060	-0.604617
22	1	0	0.880124	2.646257	0.283772
23	1	0	2.012336	2.222247	-1.037688
24	1	0	0.214414	2.207996	-1.325279
25	6	0	2.622806	0.375513	0.861487
26	1	0	3.500785	0.202932	0.221869
27	1	0	2.663223	1.389277	1.276889
28	1	0	2.632848	-0.362164	1.675261

Table S28 Ni dimethyl complex Anti-**22**
SCF Done: E(RM06) = -1899.58850716 A.U. after 11 cycles
EUMP2 = -0.18972106697291D+04
E(CCSD)= -1897.3624959
CCSD(T)= -0.18974527487D+04

Framework group C1[X(C10H18Ni)]
Deg. of freedom 81
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.581492	-0.391150	-0.019283
2	6	0	-1.263256	0.086040	0.630440
3	6	0	-1.026384	1.505298	1.166805
4	1	0	-1.446755	-0.627725	1.449962
5	6	0	-0.524198	2.388973	0.024199
6	1	0	-1.922535	1.916120	1.668074
7	1	0	-0.239559	1.462993	1.939150
8	6	0	0.432992	1.534464	-0.774328
9	1	0	-1.355359	2.724052	-0.610591
10	1	0	-0.038586	3.302049	0.401737
11	1	0	0.171700	1.268471	-1.805454
12	6	0	-2.313573	-0.027721	-0.388332
13	6	0	-3.240920	-0.994313	-0.455395
14	1	0	-2.324620	0.736707	-1.173951
15	1	0	-3.975457	-1.031996	-1.258060
16	1	0	-3.297091	-1.781819	0.298364
17	6	0	1.749429	1.284157	-0.353693
18	6	0	2.431457	0.151614	-0.820017
19	1	0	2.099215	1.759882	0.569885
20	1	0	3.384349	-0.140286	-0.381884
21	1	0	2.236590	-0.228253	-1.827593
22	6	0	-0.026986	-2.134048	-0.542787
23	1	0	0.773593	-2.864511	-0.697295
24	1	0	-0.817965	-2.547338	0.089810
25	1	0	-0.452019	-1.798960	-1.504341
26	6	0	1.458151	-1.507017	1.291208
27	1	0	2.292808	-2.122743	0.942859
28	1	0	0.738791	-2.116442	1.847388
29	1	0	1.830850	-0.682674	1.923277

Table S29 Ni dimethyl complex Syn-**22**

SCF Done: E(RM06) = -1899.59759875 A.U. after 11 cycles

EUMP2 = -0.18972195439250D+04

E(CCSD)= -1897.3729604

CCSD(T)= -0.18974677703D+04

Framework group C1[X(C10H18Ni)]

Deg. of freedom 81

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	28	0	0.531819	-0.028619	0.099607
2	6	0	-0.968341	1.258554	0.491137
3	6	0	-2.303053	0.569177	0.710760
4	1	0	-0.628464	1.940535	1.276317
5	6	0	-2.417478	-0.637893	-0.232750
6	1	0	-2.349454	0.212369	1.749817
7	1	0	-3.153998	1.262912	0.592483
8	6	0	-1.092661	-1.353897	-0.201325
9	1	0	-3.243568	-1.294275	0.076968
10	1	0	-2.651310	-0.315165	-1.258308
11	1	0	-0.910360	-1.993048	0.665572
12	6	0	-0.576614	1.555471	-0.857857
13	6	0	0.687715	1.957546	-1.187965
14	1	0	-1.220756	1.215181	-1.671095
15	1	0	1.013237	1.983531	-2.226846
16	1	0	1.349106	2.417978	-0.457978
17	6	0	-0.189106	-1.437518	-1.266587
18	6	0	1.168138	-1.678794	-0.976622
19	1	0	-0.452872	-0.986988	-2.227047
20	1	0	1.919130	-1.562104	-1.756755
21	1	0	1.441837	-2.349234	-0.159847
22	6	0	0.543947	-0.463475	2.034503
23	1	0	1.059196	0.311414	2.613966
24	1	0	-0.473126	-0.591549	2.426716
25	1	0	1.092133	-1.411426	2.130889
26	6	0	2.460063	0.346686	0.459203
27	1	0	3.001322	0.520397	-0.479810
28	1	0	2.919653	-0.496382	0.988366
29	1	0	2.521698	1.242048	1.092609

Table S30 Ni dimethyl complex Anti-**23**

SCF Done: E(RM06) = -1899.57889894 A.U. after 14 cycles

EUMP2 = -0.18971868303576D+04

E(CCSD)= -1897.3482324

CCSD(T)= -0.18974384181D+04

Framework group C1[X(C10H18Ni)]

Deg. of freedom 81

Standard orientation:

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

1	28	0	-0.958611	0.000059	-0.065564
2	6	0	1.833869	-1.394125	-0.521045
3	6	0	2.980043	-0.715902	0.102336
4	1	0	1.760674	-1.392254	-1.614791
5	6	0	2.877660	0.872278	-0.014836
6	1	0	3.039061	-0.969189	1.171701
7	1	0	3.941570	-0.983946	-0.356666
8	6	0	1.612255	1.438843	0.480018
9	1	0	3.744305	1.266218	0.534228
10	1	0	3.014987	1.129042	-1.076055
11	1	0	1.447657	1.488897	1.562657
12	6	0	0.743208	-1.752206	0.212584
13	6	0	-0.596716	-1.952076	-0.266274
14	1	0	0.870845	-1.767607	1.303600
15	1	0	-1.252444	-2.614578	0.304245
16	1	0	-0.701367	-2.085688	-1.354137
17	6	0	0.580074	1.753471	-0.359845
18	6	0	-0.788112	1.996566	-0.003805
19	1	0	0.801191	1.712204	-1.435399
20	1	0	-1.406197	2.539535	-0.722402
21	1	0	-0.983703	2.281402	1.037318
22	6	0	-2.017509	-0.343416	1.475011
23	1	0	-2.636964	-1.243022	1.433808
24	1	0	-1.197121	-0.462821	2.201946
25	1	0	-2.622036	0.541218	1.697609
26	6	0	-2.616716	0.120468	-0.980195
27	1	0	-3.263007	0.944327	-0.664080
28	1	0	-2.221204	0.309839	-1.993094
29	1	0	-3.143464	-0.838641	-0.938393

Table S31 Ni dimethyl complex Syn-**23**

SCF Done: E(RM06) = -1899.60306621 A.U. after 18 cycles
EUMP2 = -0.18972296931162D+04
E(CORR)= -1897.3763704
CCSD(T)= -0.18974669680D+04

Framework group C1[X(C10H18Ni)]
Deg. of freedom 81
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.768993	-0.033523	0.001249
2	6	0	2.101860	-1.075932	-0.801526

3	6	0	2.777993	-0.326444	0.286863
4	1	0	2.577136	-1.090495	-1.784507
5	6	0	2.333970	1.164774	0.379226
6	1	0	2.590434	-0.804384	1.258813
7	1	0	3.866486	-0.332668	0.137274
8	6	0	0.862563	1.407402	0.510751
9	1	0	2.872146	1.611007	1.227248
10	1	0	2.704704	1.676147	-0.522732
11	1	0	0.454019	1.595553	1.508230
12	6	0	0.907425	-1.702407	-0.637915
13	6	0	0.128081	-1.684445	0.585221
14	1	0	0.470100	-2.212016	-1.501326
15	1	0	-0.613863	-2.481523	0.678170
16	1	0	0.680605	-1.534321	1.517361
17	6	0	0.117607	1.770577	-0.611097
18	6	0	-1.287876	1.840734	-0.629135
19	1	0	0.632949	1.714754	-1.576928
20	1	0	-1.802547	1.992956	-1.577006
21	1	0	-1.826885	2.194358	0.252791
22	6	0	-1.874424	-0.275986	1.572514
23	1	0	-2.263031	-1.289185	1.706452
24	1	0	-1.204759	-0.011589	2.401763
25	1	0	-2.701431	0.437487	1.486247
26	6	0	-2.286115	-0.755822	-0.948073
27	1	0	-1.921154	-0.727367	-1.988142
28	1	0	-3.216053	-0.182675	-0.869825
29	1	0	-2.453564	-1.792110	-0.629828

Table S32 Reductive elimination TS **24**

SCF Done: E(RM06) = -1822.22407902 A.U. after 12 cycles
EUMP2 = -0.18200685190472D+04
E(CCSD)= -1820.1877732
CCSD(T)= -0.18202698113D+04

Framework group C1[X(C8H16Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.388115	0.109369	-0.081889
2	6	0	-1.362716	0.013733	-0.996995
3	1	0	-1.672465	1.048794	-1.199897
4	6	0	0.598955	-1.926711	-0.068609

5	1	0	0.079375	-2.114148	0.877030
6	6	0	-2.348869	-0.704151	-0.179261
7	6	0	-3.304832	-0.142938	0.577937
8	1	0	-2.268031	-1.796808	-0.170979
9	1	0	-3.985659	-0.740339	1.181762
10	1	0	-3.443016	0.939848	0.607196
11	6	0	1.874274	-1.334944	-0.042750
12	6	0	2.176637	-0.373227	0.921890
13	1	0	2.488002	-1.375300	-0.947168
14	1	0	3.080514	0.229023	0.840900
15	1	0	1.736332	-0.438556	1.920481
16	6	0	-0.131457	1.607291	1.005145
17	1	0	0.665054	2.159218	1.511124
18	1	0	-0.892589	2.283696	0.607314
19	1	0	-0.606695	0.881915	1.694094
20	6	0	1.039442	1.718069	-0.929539
21	1	0	1.851713	2.258903	-0.437359
22	1	0	0.281046	2.407000	-1.309334
23	1	0	1.433324	1.101534	-1.758155
24	1	0	0.288501	-2.551277	-0.904381
25	1	0	-1.151251	-0.498564	-1.946631

Table S33 Reductive elimination TS **25**

SCF Done: E(RM06) = -1822.22362919 A.U. after 12 cycles
EUMP2 = -0.18200669511343D+04
E(CCSD)= -1820.1878349
CCSD(T)= -0.18202699641D+04

Framework group C1[X(C8H16Ni)]
Deg. of freedom 69
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.398578	0.125775	-0.148891
2	6	0	1.376853	0.061653	-1.015777
3	1	0	1.712740	1.099043	-1.154249
4	6	0	-0.763019	-1.862350	-0.522727
5	1	0	-1.224169	-1.728067	-1.506776
6	6	0	2.293985	-0.697717	-0.154978
7	6	0	3.205966	-0.176225	0.680967
8	1	0	2.199839	-1.788472	-0.186639
9	1	0	3.837197	-0.803293	1.308110
10	1	0	3.356649	0.902716	0.755500

11	6	0	-1.471409	-1.470414	0.625798
12	6	0	-2.312682	-0.357128	0.582213
13	1	0	-1.113122	-1.815993	1.599733
14	1	0	-2.711821	0.071936	1.500260
15	1	0	-2.865250	-0.122028	-0.331281
16	6	0	-0.831154	1.863408	-0.850143
17	1	0	-0.006723	2.550698	-1.055440
18	1	0	-1.151327	1.375937	-1.791323
19	1	0	-1.672724	2.384784	-0.386237
20	6	0	0.024058	1.426138	1.214327
21	1	0	0.372355	0.605621	1.866108
22	1	0	-0.803321	1.969011	1.677794
23	1	0	0.857917	2.093533	0.981616
24	1	0	0.006945	-2.628819	-0.469932
25	1	0	1.229417	-0.412482	-1.996383

Table S34 Reductive elimination TS **26**

SCF Done: E(RM06) = -1936.42209733 A.U. after 19 cycles
EUMP2 = -0.19339775521580D+04
E(CCSD)= -1934.1215233
CCSD(T)= -0.19342240902D+04

Framework group C1[X(C11H16Ni)]
Deg. of freedom 78
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448602	1.187224	0.112268
2	6	0	-2.081762	0.007647	-0.611633
3	6	0	-0.961530	-0.994155	1.059275
4	6	0	-0.506941	0.505397	0.996333
5	1	0	-0.131835	1.006081	1.894652
6	6	0	-2.419489	-0.891476	0.591914
7	1	0	-2.835487	-1.868802	0.306561
8	1	0	-3.078840	-0.392513	1.315503
9	6	0	-0.891669	-0.734293	-1.203216
10	1	0	-0.664304	-0.759369	-2.269096
11	6	0	-0.302434	-1.563268	-0.219642
12	1	0	-2.889193	0.258804	-1.306823
13	1	0	-0.740651	-1.525906	1.990699
14	6	0	0.921251	-2.241825	-0.348119
15	1	0	1.237218	-2.576597	-1.336308
16	1	0	1.325983	-2.795078	0.499682

17	6	0	-1.677820	2.494186	-0.086717
18	1	0	-2.417844	2.836131	-0.808689
19	1	0	-1.127458	3.259237	0.461330
20	28	0	0.964691	-0.090356	-0.184697
21	6	0	1.833711	1.607654	-0.553465
22	1	0	1.332307	2.427344	-0.028640
23	1	0	2.870879	1.870571	-0.776815
24	1	0	1.326542	1.414220	-1.528734
25	6	0	2.588151	0.372592	0.831135
26	1	0	2.164193	-0.368659	1.539471
27	1	0	3.507694	-0.029976	0.397888
28	1	0	2.792245	1.276382	1.412044

Table S35 Reductive elimination TS **27**

SCF Done: E(RM06) = -1899.58818998 A.U. after 11 cycles
EUMP2 = -0.18972071772769D+04
E(CCSD)= -1897.3604151
CCSD(T)= -0.18974507535D+04
.
Framework group C1[X(C10H18Ni)]
Deg. of freedom 81

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.558147	-0.370393	-0.037448
2	6	0	-1.274792	0.097725	0.616405
3	6	0	-1.070229	1.521279	1.157687
4	1	0	-1.493217	-0.613260	1.430838
5	6	0	-0.494040	2.403172	0.047016
6	1	0	-1.993535	1.943085	1.597362
7	1	0	-0.335056	1.479598	1.978865
8	6	0	0.466647	1.539543	-0.740224
9	1	0	-1.290363	2.771474	-0.614196
10	1	0	0.000444	3.297710	0.456355
11	1	0	0.213991	1.302288	-1.781443
12	6	0	-2.276603	-0.032931	-0.449286
13	6	0	-3.181534	-1.017433	-0.564338
14	1	0	-2.264784	0.734064	-1.232996
15	1	0	-3.872156	-1.069891	-1.404270
16	1	0	-3.261986	-1.805395	0.187189
17	6	0	1.781205	1.252634	-0.327335
18	6	0	2.441014	0.126614	-0.838090
19	1	0	2.141448	1.693069	0.609746

20	1	0	3.385754	-0.202190	-0.407951
21	1	0	2.246536	-0.201491	-1.863266
22	6	0	0.143739	-2.194396	-0.455026
23	1	0	0.933508	-2.947869	-0.515146
24	1	0	-0.747196	-2.586483	0.043641
25	1	0	-0.123017	-1.836491	-1.469940
26	6	0	1.243960	-1.499014	1.380474
27	1	0	2.176607	-2.030226	1.173872
28	1	0	0.536994	-2.144107	1.909077
29	1	0	1.441695	-0.596022	1.987105

Table S36 Reductive elimination TS **28**

SCF Done: E(RM06) = -1899.59313839 A.U. after 15 cycles
EUMP2 = -0.18971989092840D+04
E(CCSD)= -1897.3584193
CCSD(T)= -0.18974493945D+04

Framework group C1[X(C10H18Ni)]
Deg. of freedom 81
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.565511	-0.154315	0.135007
2	6	0	-0.912609	1.085944	0.609312
3	6	0	-2.231378	0.361186	0.834452
4	1	0	-0.600467	1.729411	1.438964
5	6	0	-2.394725	-0.712836	-0.244333
6	1	0	-2.195241	-0.132993	1.817639
7	1	0	-3.088201	1.058317	0.869861
8	6	0	-1.063073	-1.406653	-0.327004
9	1	0	-3.209936	-1.407399	0.004709
10	1	0	-2.655923	-0.265247	-1.214970
11	1	0	-0.856755	-2.139709	0.458245
12	6	0	-0.706793	1.704727	-0.698021
13	6	0	0.321440	2.522289	-0.999036
14	1	0	-1.385476	1.428254	-1.509174
15	1	0	0.468582	2.909602	-2.005448
16	1	0	1.037489	2.834766	-0.239274
17	6	0	-0.177717	-1.350408	-1.410070
18	6	0	1.184984	-1.622105	-1.189641
19	1	0	-0.465026	-0.778464	-2.297062
20	1	0	1.920481	-1.406670	-1.962620
21	1	0	1.477835	-2.383141	-0.462456

22	6	0	0.722862	-0.505013	2.065149
23	1	0	0.130356	0.158132	2.704707
24	1	0	0.335703	-1.530574	2.152280
25	1	0	1.767606	-0.481022	2.389154
26	6	0	2.442834	0.434673	0.241685
27	1	0	2.760943	0.782584	-0.750327
28	1	0	3.100723	-0.381947	0.562700
29	1	0	2.508045	1.256076	0.967909

Table S37 Reductive elimination TS **29**

SCF Done: E(RM06) = -1899.57375115 A.U. after 10 cycles
EUMP2 = -0.18971884953388D+04
E(CCSD)= -1897.3389840
CCSD(T)= -0.18974363664D+04

Framework group C1[X(C10H18Ni)]
Deg. of freedom 81
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.879771	0.000000	-0.000001
2	6	0	1.756730	-1.467321	-0.391744
3	6	0	2.943350	-0.790528	0.138129
4	1	0	1.680090	-1.611158	-1.475458
5	6	0	2.943343	0.790536	-0.138127
6	1	0	3.017505	-0.930013	1.226928
7	1	0	3.874072	-1.161639	-0.311914
8	6	0	1.756718	1.467321	0.391745
9	1	0	3.874062	1.161655	0.311916
10	1	0	3.017498	0.930022	-1.226927
11	1	0	1.680076	1.611158	1.475458
12	6	0	0.653346	-1.712772	0.382175
13	6	0	-0.672922	-1.987693	-0.075458
14	1	0	0.784180	-1.599859	1.467095
15	1	0	-1.351110	-2.508652	0.606662
16	1	0	-0.775504	-2.310850	-1.118992
17	6	0	0.653336	1.712773	-0.382176
18	6	0	-0.672933	1.987695	0.075456
19	1	0	0.784171	1.599862	-1.467097
20	1	0	-1.351121	2.508650	-0.606667
21	1	0	-0.775517	2.310852	1.118989
22	6	0	-2.501751	-0.007172	1.038970
23	1	0	-3.141892	-0.891231	1.087275

24	1	0	-1.762303	-0.055560	1.869551
25	1	0	-3.080592	0.914359	1.133198
26	6	0	-2.501755	0.007161	-1.038965
27	1	0	-3.141902	0.891216	-1.087268
28	1	0	-1.762310	0.055554	-1.869549
29	1	0	-3.080590	-0.914374	-1.133191

Table S38 Reductive elimination TS **30**

SCF Done: E(RM06) = -1899.59945716 A.U. after 12 cycles
EUMP2 = -0.18972473753256D+04
E(CCSD)= -1897.3737867
CCSD(T)= -0.18974690914D+04

Framework group C1[X(C10H18Ni)]
Deg. of freedom 81
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.795290	-0.013265	-0.093252
2	6	0	-2.481778	-1.090731	0.550014
3	6	0	-2.907148	-0.008530	-0.379915
4	1	0	-3.114617	-1.290448	1.416921
5	6	0	-2.199645	1.333035	-0.064056
6	1	0	-2.703994	-0.274265	-1.429822
7	1	0	-3.990607	0.157843	-0.306950
8	6	0	-0.743464	1.420394	-0.396164
9	1	0	-2.729138	2.128624	-0.612038
10	1	0	-2.340107	1.550542	1.007002
11	1	0	-0.494707	1.537153	-1.460079
12	6	0	-1.309933	-1.746999	0.423055
13	6	0	-0.332943	-1.542339	-0.644937
14	1	0	-1.039194	-2.465430	1.204142
15	1	0	0.328753	-2.405742	-0.789317
16	1	0	-0.781966	-1.259299	-1.607490
17	6	0	0.202506	1.859285	0.543865
18	6	0	1.574277	1.868202	0.266802
19	1	0	-0.121104	1.906590	1.589750
20	1	0	2.291172	2.048570	1.067469
21	1	0	1.928543	2.100581	-0.741000
22	6	0	2.375769	-0.705805	-0.970847
23	1	0	2.485949	-1.782133	-1.123585
24	1	0	1.940996	-0.256361	-1.886541
25	1	0	3.338404	-0.237777	-0.750545

26	6	0	1.934868	-0.998076	1.125033
27	1	0	1.182231	-0.727305	1.891467
28	1	0	2.913186	-0.605123	1.412045
29	1	0	1.963042	-2.085215	1.012525

Sample input file for aug-cc-pvdz
%chk=/global/u1/l/lpratt/redsox31.chk
%rwf=/global/scratch/sd/lpratt/redsox31.rwf
%Mem=15Gb
%NProcS=8
#T HF/gen stable=opt

diallyl_Ni_anti_M06_CCSDT_pvdz.com

0 1

28	0	0.000041	-0.000097	-0.000722
6	0	1.576726	-1.220850	0.230779
6	0	1.942182	0.000112	-0.368906
6	0	1.576504	1.220917	0.230941
1	0	1.695169	-2.152548	-0.319409
1	0	2.201295	0.000212	-1.431663
1	0	1.694734	2.152719	-0.319115
6	0	-1.577062	-1.220746	-0.230136
6	0	-1.941594	0.000112	0.370307
6	0	-1.576840	1.220812	-0.230298
1	0	-1.694512	-2.152636	0.319930
1	0	-2.199005	0.000212	1.433475
1	0	-1.694078	2.152807	0.319636
1	0	1.581780	-1.319551	1.320467
1	0	1.581483	1.319460	1.320644
1	0	-1.583907	-1.319082	-1.319853
1	0	-1.583610	1.318990	-1.320030

C H 0
aug-cc-pvdz
****
Ni 0
cc-pvdz
S 1 1.00
  1.516000E-02 1.000000E+00
 P 1 1.00
  1.502000E-02 1.000000E+00
 D 1 1.00
  4.067000E-02 1.000000E+00
 F 1 1.00

```
   4.083000E-01     1.000000E+00
 ****
```

After optimizing the wave function, use:

```
%chk=/global/u1/l/lpratt/redsox31.chk
%rwf=/global/scratch/sd/lpratt/redsox31.rwf
%Mem=15Gb
%NProcS=8
#T CCSD(T)=maxcycl=500/gen guess=read

diallyl_Ni_anti_M06_CCSDT_pvdz.com

0 1
          28          0       0.000041   -0.000097   -0.000722
           6          0       1.576726   -1.220850    0.230779
           6          0       1.942182    0.000112   -0.368906
           6          0       1.576504    1.220917    0.230941
           1          0       1.695169   -2.152548   -0.319409
           1          0       2.201295    0.000212   -1.431663
           1          0       1.694734    2.152719   -0.319115
           6          0      -1.577062   -1.220746   -0.230136
           6          0      -1.941594    0.000112    0.370307
           6          0      -1.576840    1.220812   -0.230298
           1          0      -1.694512   -2.152636    0.319930
           1          0      -2.199005    0.000212    1.433475
           1          0      -1.694078    2.152807    0.319636
           1          0       1.581780   -1.319551    1.320467
           1          0       1.581483    1.319460    1.320644
           1          0      -1.583907   -1.319082   -1.319853
           1          0      -1.583610    1.318990   -1.320030

C H 0
aug-cc-pvdz
****
Ni 0
cc-pvdz
S 1 1.00
   1.516000E-02     1.000000E+00
 P 1 1.00
   1.502000E-02     1.000000E+00
 D 1 1.00
   4.067000E-02     1.000000E+00
 F 1 1.00
   4.083000E-01     1.000000E+00
 ****
```