Supporting Information

Differing Reactions of Functionalized Hydrocarbons with Cp*M(NO)(alkyl)(η^3-allyl) Complexes of Molybdenum and Tungsten

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Optimized structure and final thermochemical parameters of *n*Pr**A** *endo syn*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.150822	2.173276	-0.178084
2	1	0	-0.396136	2.530468	-0.884493
3	6	0	-0.738150	1.909676	1.121179
4	1	0	-1.479490	1.661734	1.878205
5	6	0	0.689763	1.780862	1.415044
6	1	0	1.339731	2.522022	0.945619
7	6	0	-1.417027	-0.772861	-0.918245
8	1	0	-1.682163	-0.138232	-1.779982
9	1	0	-1.083412	-1.736065	-1.341036
10	6	0	-2.674332	-1.057266	-0.063449
11	6	0	1.362373	-0.628450	-2.029991
12	6	0	1.788159	-1.540653	-1.000315
13	6	0	2.625080	-0.800300	-0.080937
14	6	0	2.704299	0.552305	-0.553693
15	6	0	1.923330	0.661190	-1.754492
16	7	0	-0.027770	-1.018738	1.557267
17	8	0	-0.204602	-1.787121	2.525967
18	74	0	0.385486	-0.019295	0.147894
19	1	0	3.259358	1.350390	-0.081929
20	1	0	3.127054	-1.204906	0.786711
21	1	0	1.567096	-2.597381	-0.947454
22	1	0	0.725845	-0.875796	-2.867494
23	1	0	1.798275	1.550906	-2.356567
24	6	0	-2.582383	2.317556	-0.624762
25	1	0	-2.768383	3.353815	-0.943497
26	1	0	-2.809958	1.671285	-1.482240
27	1	0	-3.286204	2.078568	0.179194
28	1	0	0.955241	1.586131	2.452482
29	1	0	-2.425349	-1.803771	0.702002
30	1	0	-2.985530	-0.157724	0.484262
31	6	0	-3.869039	-1.568036	-0.904236
32	1	0	-3.602525	-2.487528	-1.444149
33	1	0	-4.738868	-1.790156	-0.269730
34	1	0	-4.176858	-0.821568	-1.650802

Zero-point correction=	0.286483 (Hartree/Particle)
Thermal correction to Energy=	0.303928
Thermal correction to Enthalpy=	0.304872
Thermal correction to Gibbs Free Energy=	0.240995
Sum of electronic and zero-point Energies=	-666.102306
Sum of electronic and thermal Energies=	-666.084860
Sum of electronic and thermal Enthalpies=	-666.083916
Sum of electronic and thermal Free Energies=	-666.147793

Optimized structure and final thermochemical parameters of *n*Pr**A** *exo syn*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863836	2.050746	0.966872
2	1	0	0.564534	2.094190	2.013676
3	6	0	-0.137371	2.372675	-0.039171
4	1	0	0.190495	2.784987	-0.994703
5	6	0	-1.471985	2.016148	0.101093
6	1	0	-1.833059	1.740339	1.091664
7	6	0	-1.466347	-0.826120	-0.797183
8	1	0	-1.761455	-0.237351	-1.682023
9	1	0	-1.145893	-1.807091	-1.185547
10	6	0	1.324273	-1.062454	-1.878335
11	6	0	1.575393	-1.845156	-0.691752
12	6	0	2.487043	-1.095210	0.143625
13	6	0	2.763815	0.144459	-0.520398
14	6	0	2.045816	0.164741	-1.769985
15	7	0	-0.108540	-0.542875	1.750039
16	8	0	-0.338344	-1.008589	2.886312
17	74	0	0.380115	0.019058	0.138201
18	1	0	3.413112	0.923867	-0.149387
19	1	0	2.898354	-1.420776	1.088725
20	1	0	1.202727	-2.839427	-0.489536
21	1	0	0.685724	-1.351442	-2.700753
22	1	0	2.067372	0.958953	-2.503559
23	6	0	-2.512906	2.268960	-0.959834
24	1	0	-2.056321	2.553953	-1.915604
25	1	0	-3.145591	1.389895	-1.128765
26	1	0	-3.178817	3.085735	-0.643476
27	1	0	1.860552	2.449601	0.795216
28	6	0	-2.700367	-1.090841	0.099185
29	1	0	-2.400221	-1.720390	0.947395
30	1	0	-3.075647	-0.157176	0.539907
31	6	0	-3.854956	-1.782457	-0.664567
32	1	0	-4.713157	-1.974256	-0.005047
33	1	0	-4.204560	-1.162125	-1.502917
34	1	0	-3.527611	-2.745899	-1.080230

Zero-point correction=	0.286374 (Hartree/Particle)
Thermal correction to Energy=	0.303912
Thermal correction to Enthalpy=	0.304856
Thermal correction to Gibbs Free Energy=	0.240206
Sum of electronic and zero-point Energies=	-666.100190
Sum of electronic and thermal Energies=	-666.082652
Sum of electronic and thermal Enthalpies=	-666.081708
Sum of electronic and thermal Free Energies=	-666.146358

Optimized structure and final thermochemical parameters of *n*Pr**A** *endo anti*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.831618	2.173479	0.334939
2	6	0	-0.412626	1.653887	1.569140
3	1	0	-1.167580	1.290587	2.262259
4	6	0	0.975171	1.292201	1.782804
5	1	0	1.744915	1.964953	1.405556
6	6	0	-1.623957	-0.226733	-1.028430
7	1	0	-1.698420	0.593405	-1.761579
8	1	0	-1.500738	-1.154873	-1.611984
9	6	0	1.161610	-0.524145	-2.106431
10	6	0	1.301168	-1.703060	-1.289411
11	6	0	2.256722	-1.401826	-0.248936
12	6	0	2.688198	-0.045469	-0.429802
13	6	0	2.015347	0.496554	-1.577998
14	7	0	-0.412901	-1.261614	1.339435
15	8	0	-0.793129	-2.149697	2.129842
16	74	0	0.270930	-0.122413	0.158734
17	1	0	3.404737	0.473473	0.190805
18	1	0	2.599981	-2.085768	0.514673
19	1	0	0.816670	-2.655821	-1.450616
20	1	0	0.521683	-0.429718	-2.972135
21	1	0	2.141678	1.491321	-1.980832
22	1	0	1.229938	0.831689	2.734562
23	6	0	-0.042778	3.120475	-0.557478
24	1	0	-0.426395	4.141809	-0.405180
25	1	0	1.028236	3.134907	-0.335255
26	1	0	-0.176792	2.885148	-1.620263
27	1	0	-1.904268	2.198774	0.160599
28	6	0	-2.952982	-0.349787	-0.247067
29	1	0	-2.923200	-1.253204	0.376211
30	1	0	-3.081766	0.492262	0.449939
31	6	0	-4.187408	-0.410688	-1.178308
32	1	0	-4.115645	-1.263064	-1.868308
33	1	0	-5.117530	-0.520514	-0.602899
34	1	0	-4.270051	0.502757	-1.784761

Zero-point correction=	0.286973 (Hartree/Particle)
Thermal correction to Energy=	0.304322
Thermal correction to Enthalpy=	0.305266
Thermal correction to Gibbs Free Energy=	0.241830
Sum of electronic and zero-point Energies=	-666.098374
Sum of electronic and thermal Energies=	-666.081024
Sum of electronic and thermal Enthalpies=	-666.080080
Sum of electronic and thermal Free Energies=	-666.143516

Optimized structure and final thermochemical parameters of *n*Pr**A** *exo anti*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728170	-2.175523	-0.681313
2	1	0	-0.486104	-2.920914	0.074499
3	6	0	0.337238	-1.697785	-1.557823
4	1	0	0.068762	-1.289896	-2.533198
5	6	0	1.658257	-1.568605	-1.138980
6	6	0	1.225314	1.367824	-0.599684
7	1	0	1.356158	1.302170	-1.695483
8	1	0	0.793695	2.364140	-0.413123
9	6	0	-1.760151	1.806326	-0.819318
10	6	0	-1.656710	1.819631	0.621756
11	6	0	-2.344335	0.653865	1.123546
12	6	0	-2.815045	-0.090660	-0.005848
13	6	0	-2.458803	0.629295	-1.207153
14	7	0	0.453609	-0.566366	1.544890
15	8	0	0.932437	-0.868154	2.661566
16	74	0	-0.348898	-0.084413	0.039809
17	1	0	-3.364631	-1.019337	0.039223
18	1	0	-2.480844	0.393488	2.163735
19	1	0	-1.207144	2.597382	1.222892
20	1	0	-1.348842	2.549733	-1.487551
21	1	0	-2.689186	0.326888	-2.219828
22	1	0	-1.687847	-2.358074	-1.159789
23	1	0	2.323015	-0.995536	-1.784941
24	6	0	2.338780	-2.366469	-0.051399
25	1	0	2.881779	-1.726829	0.653643
26	1	0	1.641567	-2.977380	0.526598
27	1	0	3.077849	-3.033910	-0.521588
28	6	0	2.611270	1.356299	0.088216
29	1	0	2.477792	1.398319	1.178177
30	1	0	3.139832	0.416319	-0.114819
31	6	0	3.506927	2.535095	-0.362491
32	1	0	3.034224	3.499353	-0.127981
33	1	0	4.485509	2.509416	0.137766
34	1	0	3.680670	2.505246	-1.447885

Zero-point correction=	0.286600 (Hartree/Particle)
Thermal correction to Energy=	0.304174
Thermal correction to Enthalpy=	0.305118
Thermal correction to Gibbs Free Energy=	0.240794
Sum of electronic and zero-point Energies=	-666.096067
Sum of electronic and thermal Energies=	-666.078493
Sum of electronic and thermal Enthalpies=	-666.077549
Sum of electronic and thermal Free Energies=	-666.141873

Optimized structure and final thermochemical parameters of *endo* CpW(NO)(*n*-propyl)-(Me_2CHCCH_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.919078	1.859772	0.341865
2	6	0	-1.195368	1.321694	1.387899
3	1	0	-1.723876	0.657991	2.069848
4	6	0	0.257586	1.503600	1.617671
5	1	0	0.667183	2.465789	1.301456
6	6	0	-1.129628	-0.975468	-1.072234
7	1	0	-1.598239	-0.194793	-1.701081
8	1	0	-0.626189	-1.660557	-1.776021
9	6	0	-2.226075	-1.791088	-0.343893
10	6	0	1.588014	-0.037947	-2.060262
11	6	0	2.195892	-1.015358	-1.193209
12	6	0	2.838838	-0.300113	-0.111868
13	6	0	2.606683	1.100273	-0.316637
14	6	0	1.835425	1.262379	-1.519460
15	7	0	0.354065	-1.379854	1.388964
16	8	0	0.401350	-2.308189	2.227680
17	74	0	0.480735	-0.109518	0.160731
18	1	0	2.956072	1.895104	0.326877
19	1	0	3.409789	-0.744874	0.691140
20	1	0	2.222838	-2.084691	-1.349304
21	1	0	1.033012	-0.254212	-2.962096
22	1	0	1.511300	2.200771	-1.947782
23	6	0	-3.378585	1.513890	0.147218
24	1	0	-3.987193	2.428355	0.093923
25	1	0	-3.526308	0.977663	-0.802669
26	1	0	-3.767111	0.885592	0.954395
27	1	0	0.582013	1.249751	2.627547
28	1	0	-1.753620	-2.630126	0.183858
29	1	0	-2.710099	-1.183322	0.432436
30	6	0	-3.308974	-2.336585	-1.304988
31	1	0	-2.858632	-2.974160	-2.078914
32	1	0	-4.057053	-2.936512	-0.767466
33	1	0	-3.835927	-1.517423	-1.816074
34	6	0	-1.391886	2.907829	-0.620452
35	1	0	-1.979582	3.831258	-0.505200
36	1	0	-0.340210	3.154837	-0.459290
37	1	0	-1.518878	2.585120	-1.663751

Zero-point correction=	0.314220 (Hartree/Particle)
Thermal correction to Energy=	0.333330
Thermal correction to Enthalpy=	0.334274
Thermal correction to Gibbs Free Energy=	0.266561
Sum of electronic and zero-point Energies=	-705.381571
Sum of electronic and thermal Energies=	-705.362461
Sum of electronic and thermal Enthalpies=	-705.361517
Sum of electronic and thermal Free Energies=	-705.429230

Optimized structure and final thermochemical parameters of *n*Pr**TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	74	0	-0.178128	0.053584	0.021045
2	7	0	0.168225	-0.767098	1.554409
3	8	0	0.407301	-1.221553	2.694347
4	6	0	-0.126320	2.180955	-1.400577
5	1	0	0.080360	2.161494	-2.462236
6	6	0	-1.399459	2.033332	-0.787643
7	1	0	-2.342798	1.903729	-1.298764
8	6	0	-1.213430	2.092453	0.653234
9	1	0	-1.999161	2.071277	1.395259
10	6	0	0.179644	2.369425	0.901991
11	1	0	0.635970	2.484770	1.875588
12	6	0	0.850894	2.378772	-0.351041
13	1	0	1.912182	2.513565	-0.500928
14	6	0	-1.228867	-1.537069	-1.017309
15	1	0	-1.588230	-1.153710	-1.985676
16	6	0	-2.317074	-1.497532	0.015756
17	1	0	-2.189453	-2.179898	0.858573
18	6	0	-3.395962	-0.661427	0.023332
19	1	0	-3.610138	0.007090	-0.807937
20	1	0	-4.110407	-0.670330	0.842794
21	6	0	-0.588534	-2.926533	-1.189360
22	1	0	-1.320709	-3.658807	-1.562165
23	1	0	-0.189657	-3.301418	-0.237423
24	1	0	0.240092	-2.893329	-1.907796
25	6	0	1.796988	-0.421317	-0.738030
26	1	0	1.671048	-1.501074	-0.930822
27	1	0	1.972666	0.067462	-1.709743
28	6	0	3.033994	-0.243458	0.172970
29	1	0	3.167726	0.818361	0.428856
30	1	0	2.863990	-0.768888	1.121839
31	6	0	4.334224	-0.769022	-0.478903
32	1	0	4.253314	-1.841499	-0.702944
33	1	0	4.544808	-0.245410	-1.422260
34	1	0	5.197328	-0.627929	0.186299

Zero-point correction=	0.284676 (Hartree/Particle)
Thermal correction to Energy=	0.301997
Thermal correction to Enthalpy=	0.302941
Thermal correction to Gibbs Free Energy=	0.238958
Sum of electronic and zero-point Energies=	-666.082188
Sum of electronic and thermal Energies=	-666.064867
Sum of electronic and thermal Enthalpies=	-666.063923
Sum of electronic and thermal Free Energies=	-666.127906

Optimized structure and final thermochemical parameters of *n*Pr**B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.734377	-1.852285	-0.227480
2	1	0	-4.217574	-1.251194	-0.997937
3	6	0	-2.386335	-1.920565	-0.115357
4	1	0	-1.952006	-2.543147	0.670174
5	6	0	-1.411741	-1.176811	-0.963472
6	1	0	-1.929522	-0.676858	-1.791279
7	6	0	2.142905	0.218636	-0.460582
8	1	0	2.282121	0.515280	-1.518151
9	1	0	2.524396	1.062940	0.138762
10	6	0	3.034943	-1.008840	-0.147785
11	6	0	0.230065	2.584123	-0.450756
12	6	0	-0.029727	2.316848	0.942887
13	6	0	-1.376395	1.795029	1.045754
14	6	0	-1.914054	1.718678	-0.280658
15	6	0	-0.922719	2.205873	-1.204101
16	7	0	0.195355	-0.863895	1.455177
17	8	0	0.286013	-1.471891	2.544131
18	74	0	-0.007221	0.151771	0.015535
19	1	0	-2.895620	1.344450	-0.534279
20	1	0	-1.887725	1.530122	1.960399
21	1	0	0.628835	2.534398	1.772066
22	1	0	1.149966	2.982915	-0.854589
23	1	0	-1.033108	2.275387	-2.277930
24	6	0	-0.200657	-1.986146	-1.479346
25	1	0	0.777223	-1.445675	-1.350409
26	1	0	-0.082095	-2.931840	-0.944445
27	1	0	-0.261106	-2.166338	-2.558584
28	1	0	-4.388666	-2.400372	0.445562
29	1	0	2.898350	-1.298500	0.902765
30	1	0	2.724981	-1.879520	-0.746868
31	6	0	4.533593	-0.738142	-0.417064
32	1	0	4.897828	0.092983	0.202689
33	1	0	5.145942	-1.621820	-0.189500
34	1	0	4.703564	-0.470234	-1.469550

Zero-point correction= 0.284560 (Hartree/Particle)
Thermal correction to Energy= 0.302694
Thermal correction to Enthalpy= 0.303639
Thermal correction to Gibbs Free Energy= 0.237349
Sum of electronic and zero-point Energies= -666.084355
Sum of electronic and thermal Energies= -666.066221
Sum of electronic and thermal Enthalpies= -666.065277
Sum of electronic and thermal Free Energies= -666.131566

Optimized structure and final thermochemical parameters of *n*Pr**TS2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.503518	-2.381252	-0.165600
2	1	0	-4.169962	-1.785057	-0.788671
3	1	0	-3.969759	-3.122115	0.478524
4	6	0	-2.160187	-2.211420	-0.189943
5	1	0	-1.534571	-2.833399	0.453259
6	6	0	-1.444525	-1.215785	-1.025030
7	1	0	-2.103377	-0.691394	-1.721239
8	6	0	-0.092417	-1.500861	-1.556627
9	1	0	0.353438	-2.455979	-1.276482
10	1	0	0.079542	-1.250482	-2.605597
11	1	0	1.128882	-0.625531	-1.033586
12	74	0	-0.080949	0.180119	0.006807
13	7	0	0.182581	-0.856878	1.427769
14	8	0	0.333982	-1.480815	2.500635
15	6	0	-1.041067	2.164281	-1.159960
16	1	0	-1.205876	2.206449	-2.227974
17	6	0	-1.982852	1.695604	-0.169918
18	1	0	-2.975709	1.315343	-0.363050
19	6	0	-1.390362	1.851496	1.127568
20	1	0	-1.855852	1.613122	2.073708
21	6	0	-0.065337	2.396457	0.945688
22	1	0	0.626681	2.656709	1.734831
23	6	0	0.135113	2.596129	-0.467425
24	1	0	1.027292	3.002493	-0.925267
25	6	0	2.242242	0.148300	-0.515295
26	1	0	2.442263	0.866050	0.288947
27	1	0	2.492978	0.643877	-1.465222
28	6	0	3.138140	-1.095607	-0.287226
29	1	0	2.830417	-1.586376	0.645342
30	1	0	2.985372	-1.829187	-1.093600
31	6	0	4.636595	-0.730234	-0.216879
32	1	0	4.832639	-0.034662	0.610457
33	1	0	5.252316	-1.625210	-0.056547
34	1	0	4.972642	-0.251418	-1.147131

Zero-point correction=	0.281509 (Hartree/Particle)
Thermal correction to Energy=	0.298905
Thermal correction to Enthalpy=	0.299850
Thermal correction to Gibbs Free Energy=	0.234852
Sum of electronic and zero-point Energies=	-666.060847
Sum of electronic and thermal Energies=	-666.043451
Sum of electronic and thermal Enthalpies=	-666.042506
Sum of electronic and thermal Free Energies=	-666.107504

Optimized structure and final thermochemical parameters of *n*Pr**C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.546907	-1.231474	-1.011343
2	1	0	-2.330932	-0.720424	-1.575193
3	6	0	-2.057376	-2.356874	-0.195707
4	1	0	-1.302244	-2.958128	0.314175
5	6	0	-3.365488	-2.673768	-0.042273
6	1	0	-4.155970	-2.104854	-0.531430
7	6	0	2.677859	0.327282	-0.522261
8	1	0	3.105997	1.092672	-1.183385
9	1	0	2.576431	0.755319	0.479323
10	6	0	3.528290	-0.958270	-0.489668
11	6	0	-0.209681	2.614480	-0.554734
12	6	0	-0.110750	2.428032	0.877909
13	6	0	-1.325651	1.790069	1.317703
14	6	0	-2.137294	1.531137	0.160717
15	6	0	-1.449566	2.070927	-0.998706
16	7	0	0.238845	-0.896387	1.323194
17	8	0	0.494819	-1.568066	2.348018
18	74	0	-0.156533	0.190281	-0.029279
19	1	0	-3.117975	1.078157	0.166326
20	1	0	-1.574923	1.531676	2.337613
21	1	0	0.689054	2.780039	1.514542
22	1	0	0.536238	3.086536	-1.181798
23	1	0	-1.816413	2.061720	-2.015989
24	6	0	-0.217778	-1.270314	-1.654794
25	1	0	-0.153340	-0.871582	-2.669873
26	1	0	0.386158	-2.168143	-1.514110
27	1	0	-3.677598	-3.512375	0.574800
28	1	0	1.688080	0.073042	-1.004440
29	1	0	3.044956	-1.690635	0.169234
30	1	0	3.561605	-1.403415	-1.493913
31	6	0	4.964431	-0.680597	0.003559
32	1	0	5.555351	-1.604903	0.024289
33	1	0	5.480381	0.034324	-0.652422
34	1	0	4.957585	-0.264365	1.019974

Zero-point correction=	0.284460 (Hartree/Particle)
Thermal correction to Energy=	0.302881
Thermal correction to Enthalpy=	0.303825
Thermal correction to Gibbs Free Energy=	0.235246
Sum of electronic and zero-point Energies=	-666.076208
Sum of electronic and thermal Energies=	-666.057788
Sum of electronic and thermal Enthalpies=	-666.056843
Sum of electronic and thermal Free Energies=	-666.125422

Optimized structure and final thermochemical parameters of *n*Pr**H**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.937128	-1.211614	0.300469
2	1	0	3.791182	-1.803573	1.200891
3	1	0	4.890060	-0.698904	0.200627
4	6	0	2.973503	-1.104966	-0.648468
5	1	0	3.135044	-0.483859	-1.529156
6	6	0	1.678064	-1.772919	-0.546664
7	1	0	1.560312	-2.458638	0.293113
8	6	0	0.702548	-1.769761	-1.566416
9	1	0	0.939915	-1.330465	-2.529471
10	1	0	-0.023217	-2.576881	-1.592354
11	1	0	0.542824	0.577361	-1.426659
12	74	0	-0.254255	-0.126903	-0.109185
13	7	0	1.003863	0.113409	1.145562
14	8	0	1.813830	0.211645	2.083830
15	6	0	-2.336191	-1.324903	-0.810718
16	1	0	-2.434340	-1.737567	-1.805062
17	6	0	-1.812684	-2.013667	0.354389
18	1	0	-1.457211	-3.035401	0.379829
19	6	0	-1.932238	-1.145084	1.481648
20	1	0	-1.630453	-1.371023	2.495416
21	6	0	-2.433235	0.110117	1.012639
22	1	0	-2.629094	0.982057	1.619066
23	6	0	-2.716751	-0.016484	-0.403118
24	1	0	-3.144052	0.751668	-1.031423
25	6	0	-0.526160	2.080332	-0.228612
26	1	0	-1.020902	2.377855	0.711237
27	1	0	-1.225794	2.310466	-1.048091
28	6	0	0.740846	2.948358	-0.396745
29	1	0	1.473330	2.688052	0.378560
30	1	0	1.216055	2.716228	-1.360012
31	6	0	0.431878	4.461951	-0.323891
32	1	0	1.342374	5.062168	-0.458356
33	1	0	-0.284251	4.757197	-1.103541
34	1	0	-0.004881	4.728930	0.648466

Zero-point correction=	0.282986 (Hartree/Particle)
Thermal correction to Energy=	0.299995
Thermal correction to Enthalpy=	0.300939
Thermal correction to Gibbs Free Energy=	0.237757
Sum of electronic and zero-point Energies=	-666.054417
Sum of electronic and thermal Energies=	-666.037408
Sum of electronic and thermal Enthalpies=	-666.036464
Sum of electronic and thermal Free Energies=	-666.099646

Optimized structure and final thermochemical parameters of *i*Pr**A**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.237192	-0.012440	-1.553516
2	1	0	1.738838	0.733629	-2.178607
3	6	0	1.582431	-1.201104	-1.317618
4	1	0	2.087771	-1.980958	-0.750159
5	6	0	0.186685	-1.411949	-1.743502
6	1	0	-0.066374	-0.952286	-2.702078
7	6	0	0.967774	1.009590	1.385273
8	1	0	0.205176	1.241825	2.151970
9	6	0	2.067718	0.198905	2.115729
10	6	0	-1.696939	1.861696	0.232910
11	6	0	-2.363184	0.710148	0.777116
12	6	0	-2.674350	-0.173903	-0.326339
13	6	0	-2.199844	0.447052	-1.530355
14	6	0	-1.590113	1.699898	-1.187866
15	7	0	-0.261751	-1.569594	1.094682
16	8	0	-0.365691	-2.533693	1.884455
17	74	0	-0.316915	-0.181072	-0.005174
18	1	0	-2.285726	0.032954	-2.524691
19	1	0	-3.202274	-1.114553	-0.255189
20	1	0	-2.634489	0.554027	1.811750
21	1	0	-1.341790	2.707164	0.803080
22	1	0	-1.148770	2.406302	-1.877650
23	6	0	3.687180	0.247568	-1.229907
24	1	0	4.286728	0.153737	-2.149421
25	1	0	3.853795	1.261150	-0.848375
26	1	0	4.078462	-0.470501	-0.501306
27	1	0	-0.168124	-2.440588	-1.679677
28	1	0	1.648273	-0.664118	2.644251
29	1	0	2.830167	-0.176131	1.422251
30	6	0	1.556288	2.358967	0.893448
31	1	0	0.869031	2.937743	0.263731
32	1	0	1.835585	2.993751	1.751369
33	1	0	2.471315	2.194856	0.314135
34	1	0	2.586866	0.831442	2.856873

Zero-point correction=	0.285559	(Hartree/Particle)
Thermal correction to Energy=	0.303482	
Thermal correction to Enthalpy=	0.304426	
Thermal correction to Gibbs Free Energy=	0.238884	
Sum of electronic and zero-point Energies=	-666.092431	
Sum of electronic and thermal Energies=	-666.074507	
Sum of electronic and thermal Enthalpies=	-666.073563	
Sum of electronic and thermal Free Energies=	-666.139105	

Optimized structure and final thermochemical parameters of *i*Pr**TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	74	0	0.119634	0.037912	0.102670
2	7	0	-0.542140	0.344831	1.716075
3	8	0	-0.883612	0.543451	2.902177
4	6	0	1.982407	-0.979583	-1.367555
5	1	0	1.811232	-1.349654	-2.368817
6	6	0	2.313825	0.354557	-1.010260
7	1	0	2.459130	1.176780	-1.695226
8	6	0	2.447687	0.416813	0.434630
9	1	0	2.754117	1.280895	1.007137
10	6	0	2.277421	-0.920841	0.944357
11	1	0	2.332858	-1.212421	1.984234
12	6	0	1.948547	-1.763253	-0.153053
13	1	0	1.721508	-2.817979	-0.096101
14	6	0	0.478873	3.119425	-0.606165
15	1	0	1.098133	2.924205	-1.477925
16	1	0	0.796732	3.924392	0.052043
17	6	0	-0.688497	2.442653	-0.382709
18	1	0	-1.298704	2.743640	0.471020
19	6	0	-1.188948	1.258150	-1.146457
20	1	0	-0.771326	1.229293	-2.166226
21	6	0	-2.721250	1.155345	-1.188454
22	1	0	-3.151680	1.986400	-1.768142
23	1	0	-3.151194	1.192362	-0.179516
24	1	0	-3.048866	0.220736	-1.657063
25	6	0	-1.047194	-1.840618	-0.051988
26	1	0	-0.460560	-2.585278	0.507727
27	6	0	-1.203144	-2.353330	-1.508575
28	1	0	-0.241194	-2.587506	-1.982605
29	1	0	-1.717305	-1.620713	-2.145057
30	1	0	-1.807462	-3.275557	-1.523949
31	6	0	-2.427344	-1.791742	0.654778
32	1	0	-2.329232	-1.540404	1.716376
33	1	0	-3.104770	-1.062768	0.200339
34	1	0	-2.914747	-2.778765	0.582939

Zero-point correction=	0.285274 (Hartree/Particle)
Thermal correction to Energy=	0.302419
Thermal correction to Enthalpy=	0.303364
Thermal correction to Gibbs Free Energy=	0.240718
Sum of electronic and zero-point Energies=	-666.072997
Sum of electronic and thermal Energies=	-666.055852
Sum of electronic and thermal Enthalpies=	-666.054908
Sum of electronic and thermal Free Energies=	-666.117553

Optimized structure and final thermochemical parameters of *i*Pr**B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.007935	-0.588695	-0.613145
2	1	0	-4.179091	0.147120	-1.399027
3	6	0	-2.779704	-1.107174	-0.374507
4	1	0	-2.663965	-1.847225	0.420740
5	6	0	-1.527565	-0.726009	-1.088871
6	1	0	-1.757867	-0.078129	-1.944037
7	6	0	2.224269	-0.575655	-0.181370
8	1	0	2.748795	0.109800	0.507546
9	6	0	2.572296	-2.011760	0.290154
10	6	0	1.161947	2.312363	-0.085191
11	6	0	0.586367	2.073098	1.214243
12	6	0	-0.850930	2.005651	1.049833
13	6	0	-1.136482	2.173862	-0.344130
14	6	0	0.105213	2.361433	-1.045910
15	7	0	-0.177565	-1.009497	1.472589
16	8	0	-0.407235	-1.645129	2.525122
17	74	0	0.112137	0.057300	0.088201
18	1	0	-2.123026	2.149871	-0.784245
19	1	0	-1.575361	1.868533	1.840204
20	1	0	1.117980	2.030668	2.154511
21	1	0	2.216386	2.421965	-0.294324
22	1	0	0.217614	2.519658	-2.110083
23	6	0	-0.605705	-1.891676	-1.513708
24	1	0	0.475285	-1.706295	-1.271128
25	1	0	-0.862742	-2.822129	-1.001124
26	1	0	-0.612805	-2.042181	-2.599065
27	1	0	-4.874731	-0.891722	-0.031450
28	1	0	2.259124	-2.182991	1.325974
29	1	0	2.089150	-2.781243	-0.330145
30	6	0	2.793909	-0.336344	-1.608034
31	1	0	2.650148	0.693300	-1.961753
32	1	0	3.875891	-0.546420	-1.631546
33	1	0	2.328474	-1.003562	-2.349327
34	1	0	3.659337	-2.186253	0.226092

Zero-point correction=	0.284475 (Hartree/Particle)
Thermal correction to Energy=	0.302586
Thermal correction to Enthalpy=	0.303530
Thermal correction to Gibbs Free Energy=	0.238004
Sum of electronic and zero-point Energies=	-666.080509
Sum of electronic and thermal Energies=	-666.062397
Sum of electronic and thermal Enthalpies=	-666.061453
Sum of electronic and thermal Free Energies=	-666.126980

Optimized structure and final thermochemical parameters of *i*Pr**TS2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	74	0	0.047729	0.107930	0.078891
2	7	0	-0.301780	-0.933278	1.476599
3	8	0	-0.549026	-1.551262	2.535036
4	6	0	0.103106	2.312382	-1.092523
5	1	0	0.153506	2.421682	-2.167304
6	6	0	-1.100655	2.228226	-0.300216
7	1	0	-2.113821	2.247333	-0.675280
8	6	0	-0.728526	2.146408	1.082952
9	1	0	-1.406486	2.093189	1.923313
10	6	0	0.714258	2.160208	1.153578
11	1	0	1.304975	2.140720	2.059164
12	6	0	1.215724	2.273844	-0.190982
13	1	0	2.259559	2.327231	-0.469493
14	6	0	-4.025358	-0.970718	-0.649191
15	1	0	-4.324650	-0.179201	-1.336005
16	1	0	-4.820959	-1.467796	-0.100472
17	6	0	-2.727803	-1.321251	-0.484194
18	1	0	-2.478555	-2.120840	0.216239
19	6	0	-1.580393	-0.686007	-1.177775
20	1	0	-1.890306	0.031583	-1.941741
21	6	0	-0.376793	-1.475369	-1.533442
22	1	0	0.015205	-1.326690	-2.541122
23	1	0	-0.373526	-2.523868	-1.233130
24	1	0	0.972221	-1.125497	-0.815180
25	6	0	2.256238	-0.827157	-0.140067
26	1	0	2.610962	-0.119531	0.618860
27	6	0	3.043908	-0.583025	-1.450784
28	1	0	2.899681	0.432415	-1.840563
29	1	0	2.741475	-1.287319	-2.239014
30	1	0	4.120461	-0.729356	-1.279823
31	6	0	2.482843	-2.256556	0.406072
32	1	0	1.969480	-2.403746	1.361767
33	1	0	3.557282	-2.438395	0.558250
34	1	0	2.116912	-3.021625	-0.293466

Zero-point correction=	0.281603 (Hartree/Particle)
Thermal correction to Energy=	0.298932
Thermal correction to Enthalpy=	0.299876
Thermal correction to Gibbs Free Energy=	0.236160
Sum of electronic and zero-point Energies=	-666.058799
Sum of electronic and thermal Energies=	-666.041470
Sum of electronic and thermal Enthalpies=	-666.040526
Sum of electronic and thermal Free Energies=	-666.104241

Optimized structure and final thermochemical parameters of *i*Pr**C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.693385	-0.746073	-1.162179
2	1	0	-2.203720	0.000898	-1.774758
3	6	0	-2.624734	-1.667311	-0.473044
4	1	0	-2.163910	-2.488959	0.078419
5	6	0	-3.974796	-1.554700	-0.479922
6	1	0	-4.481952	-0.753445	-1.017104
7	6	0	2.772914	-0.734015	-0.084647
8	1	0	2.771185	-0.241615	0.893251
9	6	0	2.901043	-2.257719	0.092465
10	6	0	0.710597	2.454992	-0.442710
11	6	0	0.646391	2.241327	0.989848
12	6	0	-0.736038	2.032079	1.336015
13	6	0	-1.506659	2.045843	0.123495
14	6	0	-0.603955	2.339240	-0.975739
15	7	0	-0.175098	-1.031831	1.367021
16	8	0	-0.250524	-1.772874	2.374140
17	74	0	-0.049750	0.139049	0.034374
18	1	0	-2.578594	1.930520	0.053874
19	1	0	-1.123703	1.864626	2.331449
20	1	0	1.471540	2.318074	1.684345
21	1	0	1.608236	2.665609	-1.010105
22	1	0	-0.884031	2.445417	-2.014961
23	6	0	-0.375141	-1.192855	-1.661104
24	1	0	-0.067642	-0.812071	-2.637970
25	1	0	-0.106740	-2.239919	-1.512299
26	1	0	-4.606203	-2.263427	0.049690
27	1	0	1.790165	-0.544013	-0.620751
28	1	0	2.113188	-2.648530	0.744894
29	1	0	2.840293	-2.773631	-0.874327
30	6	0	3.857370	-0.117851	-0.991176
31	1	0	3.734304	0.967610	-1.094678
32	1	0	4.851298	-0.305013	-0.563345
33	1	0	3.833729	-0.563259	-1.993979
34	1	0	3.872289	-2.500413	0.544632

Zero-point correction=	0.284158 (Hartree/Particle)
Thermal correction to Energy=	0.302634
Thermal correction to Enthalpy=	0.303578
Thermal correction to Gibbs Free Energy=	0.235523
Sum of electronic and zero-point Energies=	-666.077509
Sum of electronic and thermal Energies=	-666.059033
Sum of electronic and thermal Enthalpies=	-666.058088
Sum of electronic and thermal Free Energies=	-666.126144

Optimized structure and final thermochemical parameters of *i*Pr**H**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.176036	-0.163179	0.015172
2	1	0	4.257123	-0.796368	0.895441
3	1	0	4.963201	0.571042	-0.134626
4	6	0	3.134092	-0.269476	-0.847313
5	1	0	3.059704	0.394224	-1.707949
6	6	0	2.059196	-1.242797	-0.671890
7	1	0	2.186057	-1.948380	0.149451
8	6	0	1.022858	-1.468508	-1.601116
9	1	0	1.053347	-0.980166	-2.569653
10	1	0	0.526095	-2.433245	-1.579646
11	1	0	0.386209	0.818238	-1.367575
12	74	0	-0.184297	-0.093403	-0.053129
13	7	0	1.064255	0.244092	1.186053
14	8	0	1.885600	0.422234	2.104806
15	6	0	-1.862314	-1.886283	-0.632169
16	1	0	-1.741706	-2.522837	-1.497212
17	6	0	-1.344864	-2.143165	0.692574
18	1	0	-0.784491	-3.015486	1.000946
19	6	0	-1.793458	-1.083556	1.550125
20	1	0	-1.590908	-0.991228	2.608407
21	6	0	-2.516490	-0.146115	0.745604
22	1	0	-2.988049	0.758712	1.098662
23	6	0	-2.575747	-0.654622	-0.605777
24	1	0	-3.082020	-0.191937	-1.440274
25	6	0	-0.737415	2.097048	0.039697
26	1	0	-1.189135	2.195031	1.043091
27	6	0	0.491435	3.038317	0.014030
28	1	0	1.227277	2.778340	0.782255
29	1	0	0.997099	2.999922	-0.959768
30	1	0	0.172428	4.080723	0.187339
31	6	0	-1.765567	2.580663	-1.010178
32	1	0	-1.386236	2.425649	-2.029437
33	1	0	-2.735233	2.072691	-0.933563
34	1	0	-1.953949	3.660405	-0.887720

Zero-point correction=	0.283047 (Hartree/Particle)
Thermal correction to Energy=	0.300739
Thermal correction to Enthalpy=	0.301683
Thermal correction to Gibbs Free Energy=	0.237233
Sum of electronic and zero-point Energies=	-666.049217
Sum of electronic and thermal Energies=	-666.031524
Sum of electronic and thermal Enthalpies=	-666.030580
Sum of electronic and thermal Free Energies=	-666.095030