Supporting information

TRIALKYLSULFONIUM AND TETRAALKYLAMMONIUM SALTS AS HYDROGEN-BONDING CATALYSTS IN AN AZA-DIELS-ALDER REACTION: EXPERIMENTAL AND COMPUTATIONAL STUDIES

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Dedicated to Professor Kaoru Fuji on the occasion of his 80th birthday

Computational details

Global Reaction Route Mapping (GRRM) method was firstly performed at the PM6 level using the simplified model system (Ar group was exchanged by Me group) to find various types of alkyl-onium catalyst/imine complexes (**CP**) without prejudice. In GRRM method, *l*-ADDF search was performed in two modes; (i) using a certain optimized structure of alkyl-onium catalyst/imine complex, or (ii) adding imine with random initial position to alkyl-onium catalyst. All alkyl-onium catalyst/imine complexes obtained by GRRM method were further reoptimized at the B3LYP/6-31+G** level. On the other hand, transition state (TS) structure of the aza-Diels-Alder reaction without catalyst was investigated at the B3LYP/6-31+G** level. Next, the optimal TS structure without catalyst (DFT) was combined with various types of alkyl-onium catalyst/imine complexes (GRRM/DFT) to systematically explore possible and stable TS conformations using the simplified model. Finally, the most promising TS structures were expanded to the realistic model (introduction of Ph groups on imine) and optimized at the dispersion corrected B3LYP-D3/6-31+G** level. Single-point energy calculations of the realistic **CP** and **TS** models optimized at the B3LYP-D3/6-31+G** level were evaluated at the B3LYP-D3/6-311+G** with solvation model based on density (SMD) of CH_2Cl_2. Frequency calculation were carried out to characterize the stationary points and to estimate

thermodynamic properties (298.15 K, 1atm) and Gibbs free energies. All DFT calculations were performed with the Gaussian 09 package.

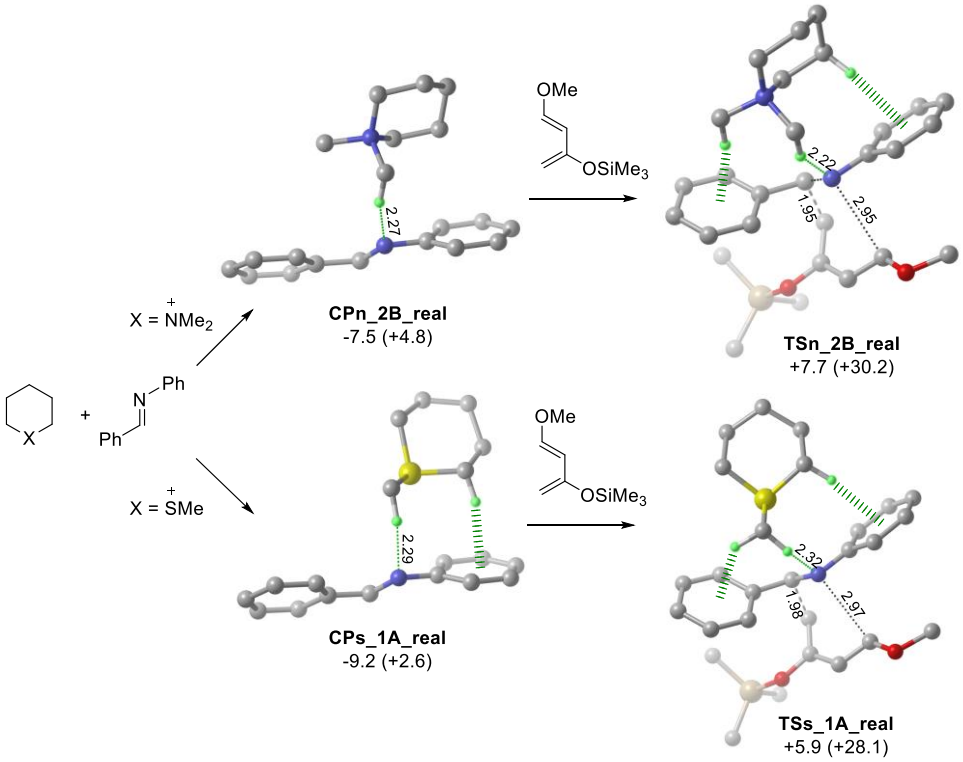

Figure S1. Three-dimensional (3D) structures and relative energies of catalyst/imine complexes **CP** and the corresponding transition state **TS** (**n**: ammonium catalyst, **s**: sulfonium catalyst) at the B3LYP/6-31+G** level [SMD(CH_2Cl_2)-B3LYP/6-311+G**// B3LYP/6-31+G** in parenthesis]. Interacting hydrogen atoms are highlighted in green (other hydrogen atoms are omitted). Hydrogen bond distances are shown in Å.

Cartesian coordinates of calculated structures

Simplified models

CPs_1A

SCF Done: E(RB3LYP) = -807.73922392 A.U.
Sum of electronic and thermal Free Energies= -807.502447 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.702318	1.735174	-0.435794
2	6	0	-0.689581	0.954638	0.409105
3	6	0	-2.521817	-1.169615	0.245503
4	6	0	-3.378832	-0.205572	-0.586084
5	6	0	-3.154477	1.273691	-0.230517
6	1	0	0.348109	1.250202	0.236849
7	1	0	-0.915897	1.009188	1.479216
8	1	0	-1.601127	2.789026	-0.153433
9	1	0	-1.426631	1.673247	-1.495798
10	1	0	-2.678900	-2.214079	-0.036078
11	1	0	-2.696529	-1.054260	1.320138
12	1	0	-3.193800	-0.374871	-1.654007
13	1	0	-4.424429	-0.479769	-0.407581
14	1	0	-3.815228	1.889804	-0.847658
15	1	0	-3.451785	1.449134	0.812042
16	16	0	-0.737900	-0.825109	-0.063556
17	6	0	3.529056	0.105666	-0.688280
18	7	0	2.744087	0.316062	0.295700
19	6	0	3.283257	1.045314	1.443415
20	1	0	4.334428	1.339526	1.318912
21	1	0	2.687685	1.949004	1.615653
22	1	0	3.199504	0.425016	2.342830
23	1	0	4.569251	0.465675	-0.661029
24	6	0	3.122194	-0.626828	-1.928091
25	1	0	3.763335	-1.504100	-2.076800
26	1	0	2.079211	-0.949206	-1.881479
27	1	0	3.261405	0.012117	-2.808525
28	6	0	0.123979	-1.655066	1.305865
29	1	0	0.054825	-2.731208	1.135550
30	1	0	1.162057	-1.318803	1.235870
31	1	0	-0.326449	-1.380753	2.261594

CPs_1B

SCF Done: E(RB3LYP) = -807.739534112 A.U.
Sum of electronic and thermal Free Energies= -807.504407 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.638700	1.777027	0.306600
2	6	0	-0.602903	0.911287	-0.418985
3	6	0	-2.541421	-1.120197	-0.289314
4	6	0	-3.411416	-0.077024	0.424557
5	6	0	-3.091466	1.369509	0.012468
6	1	0	0.430825	1.168723	-0.177159
7	1	0	-0.744789	0.922275	-1.504781
8	1	0	-1.466646	2.809640	-0.016907
9	1	0	-1.446904	1.757221	1.386553
10	1	0	-2.767292	-2.139810	0.033723
11	1	0	-2.634364	-1.057753	-1.378269
12	1	0	-3.313986	-0.195994	1.510781
13	1	0	-4.452704	-0.314970	0.180987
14	1	0	-3.766730	2.046637	0.544024
15	1	0	-3.300269	1.500567	-1.057768
16	16	0	-0.769720	-0.839050	0.132755
17	6	0	3.625999	0.422371	-0.003962
18	7	0	2.580461	-0.063404	0.543735
19	6	0	2.686566	-0.482226	1.941239
20	1	0	3.684922	-0.319521	2.370012
21	1	0	2.441349	-1.546997	2.022139
22	1	0	1.954138	0.066803	2.543297
23	1	0	4.563033	0.517640	0.566255
24	6	0	3.674845	0.890954	-1.424619
25	1	0	4.440001	0.335309	-1.980086
26	1	0	3.967941	1.946945	-1.465698
27	1	0	2.711528	0.767925	-1.925671
28	6	0	0.134177	-1.779211	-1.134805
29	1	0	-0.028776	-2.840381	-0.936063
30	1	0	1.185680	-1.519620	-0.992174
31	1	0	-0.218736	-1.510960	-2.132482

CPs_2A

SCF Done: E(RB3LYP) = -807.73829543 A.U.
Sum of electronic and thermal Free Energies= -807.503307 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.931898	-0.258409	1.760293
2	6	0	0.936979	0.734036	1.146932
3	6	0	1.581744	-0.487815	-1.303864
4	6	0	2.520957	-1.372868	-0.475251
5	6	0	2.047057	-1.573842	0.973133
6	1	0	-0.072507	0.321633	1.041644
7	1	0	0.897076	1.674980	1.702020
8	1	0	2.917163	0.213431	1.862276
9	1	0	1.581468	-0.461790	2.778333
10	1	0	0.560850	-0.880022	-1.334116
11	1	0	1.945698	-0.335142	-2.323232
12	1	0	2.578238	-2.338558	-0.989603
13	1	0	3.534722	-0.954021	-0.491579
14	1	0	1.077223	-2.088084	0.974516
15	1	0	2.750861	-2.235040	1.487483
16	16	0	1.493957	1.193576	-0.552546
17	6	0	-3.269299	-0.832041	-0.054995
18	7	0	-2.519714	0.146840	0.273236
19	6	0	-3.100323	1.179281	1.131130
20	1	0	-4.144386	0.980148	1.408747
21	1	0	-2.508477	1.268588	2.049129
22	1	0	-3.056449	2.146877	0.618558
23	1	0	-4.308964	-0.886073	0.303229
24	6	0	-2.820922	-1.959692	-0.930290
25	1	0	-3.460729	-2.028385	-1.818223
26	1	0	-1.783289	-1.831707	-1.247901
27	1	0	-2.919689	-2.914666	-0.400262
28	6	0	-0.002472	1.911669	-1.305344
29	1	0	0.173943	1.972683	-2.381312
30	1	0	-0.869265	1.288630	-1.062198
31	1	0	-0.112515	2.919512	-0.899881

CPs_2B

SCF Done: E(RB3LYP) = -807.73876683 A.U.
Sum of electronic and thermal Free Energies= -807.503363 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.895688	-0.188714	1.811346

2	6	0	0.831593	0.727496	1.194720
3	6	0	1.636536	-0.367285	-1.263870
4	6	0	2.630457	-1.190580	-0.435243
5	6	0	2.145631	-1.468183	0.996979
6	1	0	-0.130370	0.224621	1.047841
7	1	0	0.689831	1.644279	1.772984
8	1	0	2.832401	0.365688	1.948760
9	1	0	1.541227	-0.447902	2.815183
10	1	0	0.651769	-0.839294	-1.323684
11	1	0	2.007215	-0.159481	-2.270997
12	1	0	2.780206	-2.134624	-0.970789
13	1	0	3.605339	-0.687677	-0.419071
14	1	0	1.226163	-2.067001	0.963731
15	1	0	2.894533	-2.076663	1.512708
16	16	0	1.392784	1.281009	-0.474934
17	6	0	-3.382305	-0.373453	0.303731
18	7	0	-2.288880	-0.628727	-0.303162
19	6	0	-2.242613	-1.841073	-1.119204
20	1	0	-3.183611	-2.408157	-1.114127
21	1	0	-2.005292	-1.574796	-2.155628
22	1	0	-1.443156	-2.496819	-0.755243
23	1	0	-4.245430	-1.050282	0.208988
24	6	0	-3.588236	0.829069	1.170081
25	1	0	-3.859501	0.520856	2.187019
26	1	0	-2.694501	1.455900	1.212987
27	1	0	-4.426695	1.427017	0.793245
28	6	0	-0.138013	1.895289	-1.249643
29	1	0	0.072715	2.040220	-2.311354
30	1	0	-0.944131	1.172760	-1.082690
31	1	0	-0.363523	2.860902	-0.792180

CPs_3A

SCF Done: E(RB3LYP) = -807.73833801 A.U.

Sum of electronic and thermal Free Energies= -807.503640 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.445258	1.644730	-0.512277
2	6	0	-0.601129	0.474233	-1.017417
3	6	0	-2.677440	-1.138319	0.111174
4	6	0	-3.307889	0.201359	0.495750
5	6	0	-2.952249	1.348033	-0.463206
6	1	0	-0.852383	0.202843	-2.048176
7	1	0	0.479102	0.640164	-0.954778
8	1	0	-1.090030	1.971505	0.472353
9	1	0	-1.251627	2.480136	-1.195098
10	1	0	-3.031479	-1.491588	-0.863033
11	1	0	-2.869941	-1.929231	0.841781
12	1	0	-4.392291	0.041826	0.502348
13	1	0	-3.036726	0.467282	1.524366
14	1	0	-3.315767	1.111985	-1.472406
15	1	0	-3.483478	2.250975	-0.147989
16	16	0	-0.841199	-1.101333	-0.085312
17	6	0	3.631298	0.499016	0.060245
18	7	0	2.694176	-0.333097	-0.181062
19	6	0	3.065675	-1.606862	-0.796511
20	1	0	2.749287	-2.431424	-0.147899
21	1	0	2.536418	-1.719715	-1.749266
22	1	0	4.144190	-1.703276	-0.982459
23	1	0	4.674927	0.254560	-0.191310
24	6	0	3.405230	1.839306	0.686380
25	1	0	3.762303	2.633653	0.019830
26	1	0	2.348845	2.007554	0.909436
27	1	0	3.985449	1.927190	1.612769
28	6	0	-0.208424	-0.721207	1.579289
29	1	0	-0.342549	-1.619054	2.185555
30	1	0	0.855165	-0.511085	1.433199
31	1	0	-0.728339	0.126969	2.022650

CPs_3B

SCF Done: E(RB3LYP) = -807.73827229 A.U.

Sum of electronic and thermal Free Energies= -807.503025 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.638700	1.777027	0.306600
2	6	0	-0.602903	0.911287	-0.418985
3	6	0	-2.541421	-1.120197	-0.289314
4	6	0	-3.411416	-0.077024	0.424557
5	6	0	-3.091466	1.369509	0.012468
6	1	0	0.430825	1.168723	-0.177159
7	1	0	-0.744789	0.922275	-1.504781
8	1	0	-1.466646	2.809640	-0.016907
9	1	0	-1.446904	1.757221	1.386553
10	1	0	-2.767292	-2.139810	0.033723
11	1	0	-2.634364	-1.057753	-1.378269
12	1	0	-3.313986	-0.195994	1.510781
13	1	0	-4.452704	-0.314970	0.180987
14	1	0	-3.766730	2.046637	0.544024
15	1	0	-3.300269	1.500567	-1.057768
16	16	0	-0.769720	-0.839050	0.132755
17	6	0	3.625999	0.422371	-0.003962
18	7	0	2.580461	-0.063404	0.543735
19	6	0	2.686566	-0.482226	1.941239
20	1	0	3.684922	-0.319521	2.370012
21	1	0	2.441349	-1.546997	2.022139
22	1	0	1.954138	0.066803	2.543297
23	1	0	4.563033	0.517640	0.566255
24	6	0	3.674845	0.890954	-1.424619
25	1	0	4.440001	0.335309	-1.980086
26	1	0	3.967941	1.946945	-1.465698F
27	1	0	2.711528	0.767925	-1.925671
28	6	0	0.134177	-1.779211	-1.134805
29	1	0	-0.028776	-2.840381	-0.936063
30	1	0	1.185680	-1.519620	-0.992174
31	1	0	-0.218736	-1.510960	-2.132482

CPs_4

SCF Done: E(RB3LYP) = -807.73725893 A.U.

Sum of electronic and thermal Free Energies= -807.501899 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895182	1.067271	1.283590
2	6	0	-0.851193	-0.041254	1.422417
3	6	0	-0.849815	-0.041572	-1.422019
4	6	0	-1.893986	1.066900	-1.284460
5	6	0	-1.746696	1.899347	-0.000481
6	1	0	0.174228	0.341975	1.435121
7	1	0	-1.002796	-0.667973	2.305806
8	1	0	-2.907746	0.652388	1.355566
9	1	0	-1.774761	1.713738	2.160788
10	1	0	0.175644	0.341601	-1.433560
11	1	0	-1.000444	-0.668545	-2.305391
12	1	0	-1.772804	1.713143	-2.161720
13	1	0	-2.906472	0.651962	-1.357243
14	1	0	-0.771722	2.402685	-0.000108

15	1	0	-2.504300	2.688677	-0.000949
16	16	0	-0.793827	-1.216774	0.000396
17	6	0	3.352550	-0.212262	0.000186
18	7	0	2.314921	0.531002	0.000011
19	6	0	2.529006	1.977981	0.000355
20	1	0	3.590138	2.262983	-0.000074
21	1	0	2.052210	2.419451	-0.882270
22	1	0	2.053081	2.418891	0.883738
23	1	0	4.359078	0.234156	0.000527
24	6	0	3.302286	-1.707520	-0.000109
25	1	0	3.826890	-2.103262	0.877962
26	1	0	2.274253	-2.075910	0.000145
27	1	0	3.826262	-2.102839	-0.878758
28	6	0	-2.440243	-2.000007	-0.000275
29	1	0	-2.494573	-2.629824	-0.890499
30	1	0	-2.495354	-2.629766	0.889940
31	1	0	-3.244391	-1.265461	-0.000659

CPs_5

SCF Done: E(RB3LYP) = -807.7322605 A.U.

Sum of electronic and thermal Free Energies= -807.497817 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.547553	-1.639060	-0.286930
2	6	0	0.650830	-0.513649	-0.796054
3	6	0	2.684363	0.847616	0.692612
4	6	0	3.472909	0.096506	-0.384455
5	6	0	3.052563	-1.383911	-0.534183
6	1	0	0.847196	-0.262832	-1.842315
7	1	0	-0.423078	-0.693854	-0.681090
8	1	0	1.353301	-1.807670	0.779070
9	1	0	1.237652	-2.560997	-0.790568
10	1	0	3.062836	1.857964	0.861754
11	1	0	2.657718	0.309432	1.644119
12	1	0	3.377583	0.630741	-1.337613
13	1	0	4.532811	0.160230	-0.118011
14	1	0	3.323959	-1.720602	-1.539716
15	1	0	3.627180	-2.002801	0.162278
16	16	0	0.932639	1.071378	0.124192
17	6	0	-3.727254	-0.450073	-0.033576
18	7	0	-2.743983	0.288725	-0.374225
19	6	0	-3.006458	1.362738	-1.331382
20	1	0	-4.055961	1.414242	-1.652430
21	1	0	-2.731178	2.324845	-0.885130
22	1	0	-2.378290	1.222341	-2.218301
23	1	0	-4.730433	-0.274350	-0.451841
24	6	0	-3.610627	-1.585173	0.934751
25	1	0	-3.929842	-2.521284	0.461050
26	1	0	-2.587216	-1.700812	1.299671
27	1	0	-4.280217	-1.425068	1.788439
28	6	0	-0.047659	0.841540	1.641234
29	1	0	0.108073	1.722627	2.266481
30	1	0	-1.089083	0.770316	1.312125
31	1	0	0.265311	-0.064797	2.162435

CPn_1A

SCF Done: E(RB3LYP) = -504.23408063 A.U.

Sum of electronic and thermal Free Energies= -503.951725 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.885423	0.245412	1.735326
2	6	0	-1.019090	-0.733315	0.945412
3	6	0	-1.216554	0.697530	-1.089047
4	6	0	-2.081616	1.695922	-0.322539
5	6	0	-1.771961	1.672591	1.180742
6	1	0	0.039298	-0.465918	1.016486
7	1	0	-1.145624	-1.765236	1.282872
8	1	0	-2.931501	-0.082332	1.750706
9	1	0	-1.542518	0.205733	2.774670
10	1	0	-0.158212	0.954869	-0.997679
11	1	0	-1.475114	0.652661	-2.150021
12	1	0	-1.877771	2.685098	-0.746051
13	1	0	-3.146069	1.505250	-0.501370
14	1	0	-0.755888	2.050573	1.351525
15	1	0	-2.452430	2.340887	1.715962
16	6	0	3.489994	0.474050	-0.091307
17	7	0	2.585135	-0.346963	0.275034
18	6	0	2.982909	-1.423139	1.181294
19	1	0	2.397538	-1.358653	2.105687
20	1	0	2.758363	-2.391136	0.719204
21	1	0	4.049689	-1.402217	1.443800
22	1	0	4.524218	0.365754	0.271000
23	6	0	3.240359	1.622264	-1.017954
24	1	0	2.197337	1.657636	-1.341313
25	1	0	3.496892	2.569001	-0.527396
26	1	0	3.885561	1.543895	-1.901191
27	6	0	-2.688992	-1.307088	-0.831716
28	1	0	-2.854075	-1.310703	-1.909949
29	1	0	-2.718588	-2.328369	-0.450124
30	1	0	-3.456953	-0.711703	-0.344564
31	7	0	-1.326949	-0.731215	-0.554823
32	6	0	-0.294334	-1.581623	-1.251944
33	1	0	-0.387857	-2.607321	-0.891377
34	1	0	0.696716	-1.186255	-1.015530
35	1	0	-0.482071	-1.549892	-2.326432

CPn_1B

SCF Done: E(RB3LYP) = -504.23439793 A.U.

Sum of electronic and thermal Free Energies= -503.951572 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.327916	1.437998	-0.448104
2	6	0	1.407824	0.444655	-1.155230
3	6	0	0.800523	-0.591166	1.032275
4	6	0	1.714823	0.387703	1.766236
5	6	0	1.870366	1.704673	0.992964
6	1	0	0.394273	0.845225	-1.234297
7	1	0	1.763003	0.192063	-2.157565
8	1	0	3.365953	1.086339	-0.465648
9	1	0	2.313592	2.360935	-1.037509
10	1	0	-0.211403	-0.186543	0.931427
11	1	0	0.744592	-1.560000	1.535425
12	1	0	1.264165	0.567033	2.748151
13	1	0	2.694411	-0.063689	1.962715
14	1	0	0.910235	2.236133	0.980135
15	1	0	2.585890	2.357982	1.500296
16	6	0	-3.531040	0.054256	0.209367
17	7	0	-2.446418	0.499716	-0.293557
18	6	0	-2.511579	1.773706	-1.007121
19	1	0	-1.831879	2.491922	-0.534303
20	1	0	-2.174164	1.631075	-2.040195
21	1	0	-3.518769	2.212645	-1.028734
22	1	0	-4.470509	0.618751	0.102813

23	6	0	-3.625111	-1.234189	0.964972
24	1	0	-4.342783	-1.906223	0.479151
25	1	0	-2.656224	-1.734354	1.031860
26	1	0	-4.005470	-1.052563	1.977368
27	6	0	2.544060	-1.656356	-0.418795
28	1	0	2.391643	-2.593290	0.118132
29	1	0	2.812774	-1.864011	-1.455362
30	1	0	3.336269	-1.085380	0.058564
31	7	0	1.257058	-0.877652	-0.401795
32	6	0	0.189875	-1.695784	-1.084300
33	1	0	0.489470	-1.869651	-2.119088
34	1	0	-0.750735	-1.142226	-1.036783
35	1	0	0.095236	-2.649594	-0.562686

CPn_2A

SCF Done: E(RB3LYP) = -504.23459296 A.U.

Sum of electronic and thermal Free Energies= -503.951231 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.414587	1.581609	-0.621235
2	6	0	-0.735989	0.249095	-0.931702
3	6	0	-2.584009	-0.976693	0.231244
4	6	0	-3.277885	0.345994	0.551372
5	6	0	-2.935409	1.428274	-0.481849
6	1	0	-1.080405	-0.137479	-1.895699
7	1	0	0.354926	0.319638	-0.946062
8	1	0	-0.988054	2.029891	0.283594
9	1	0	-1.166743	2.263453	-1.441667
10	1	0	-2.936841	-1.370400	-0.726658
11	1	0	-2.759632	-1.733707	0.999869
12	1	0	-4.354646	0.146842	0.564174
13	1	0	-3.021042	0.681423	1.562592
14	1	0	-3.367929	1.157825	-1.454253
15	1	0	-3.387002	2.381254	-0.192011
16	6	0	3.521090	0.779127	0.093878
17	7	0	2.789150	-0.253946	-0.062807
18	6	0	3.464111	-1.511309	-0.381126
19	1	0	4.556867	-1.416979	-0.447192
20	1	0	3.226979	-2.256974	0.386343
21	1	0	3.092597	-1.893181	-1.339135
22	1	0	4.615121	0.711370	-0.010278
23	6	0	2.979637	2.135096	0.423197
24	1	0	3.262792	2.854970	-0.354230
25	1	0	1.891374	2.121788	0.518993
26	1	0	3.416910	2.500700	1.360044
27	6	0	-0.418994	-0.537257	1.416778
28	1	0	-0.633671	-1.358026	2.102733
29	1	0	0.655993	-0.442792	1.246170
30	1	0	-0.819425	0.389250	1.820777
31	7	0	-1.070080	-0.842606	0.089409
32	6	0	-0.508284	-2.147042	-0.409003
33	1	0	0.572006	-2.041298	-0.505197
34	1	0	-0.953151	-2.380014	-1.376952
35	1	0	-0.748601	-2.933046	0.308500

CPn_2B

SCF Done: E(RB3LYP) = -504.23422000 A.U.

Sum of electronic and thermal Free Energies= -503.950913 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.538047	1.437359	-0.876844
2	6	0	-0.714706	0.151586	-0.900215
3	6	0	-2.556474	-1.060714	0.289392
4	6	0	-3.393362	0.216326	0.322774
5	6	0	-3.045714	1.150871	-0.844444
6	1	0	-0.923720	-0.418094	-1.810853
7	1	0	0.361654	0.333732	-0.831693
8	1	0	-1.246793	2.066413	-0.027844
9	1	0	-1.269752	2.002173	-1.776059
10	1	0	-2.773296	-1.635977	-0.615617
11	1	0	-2.741851	-1.700642	1.155939
12	1	0	-4.444007	-0.089253	0.277475
13	1	0	-3.270509	0.732875	1.281566
14	1	0	-3.351745	0.685759	-1.790915
15	1	0	-3.607126	2.085466	-0.758282
16	6	0	3.766315	0.104173	-0.203533
17	7	0	2.659984	0.581101	0.216193
18	6	0	2.692588	1.913022	0.818993
19	1	0	3.694785	2.363326	0.830848
20	1	0	2.019478	2.579736	0.268114
21	1	0	2.326910	1.857583	1.850763
22	1	0	4.697581	0.683832	-0.106835
23	6	0	3.901588	-1.241357	-0.844053
24	1	0	4.584598	-1.871204	-0.261226
25	1	0	2.936786	-1.746240	-0.930811
26	1	0	4.343486	-1.143230	-1.842763
27	6	0	-0.571905	-0.216630	1.565878
28	1	0	-0.794589	-0.929308	2.361314
29	1	0	0.503985	-0.055269	1.481364
30	1	0	-1.078444	0.724183	1.766168
31	7	0	-1.053501	-0.793984	0.257807
32	6	0	-0.329370	-2.094837	0.038261
33	1	0	0.741533	-1.892313	0.021339
34	1	0	-0.648608	-2.524788	-0.911609
35	1	0	-0.571206	-2.777382	0.854363

CPn_3A

SCF Done: E(RB3LYP) = -504.23478896 A.U.

Sum of electronic and thermal Free Energies= -503.952119 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.090106	1.584391	-0.347890
2	6	0	1.059316	0.894958	0.543813
3	6	0	2.325833	-1.252316	0.382292
4	6	0	3.368415	-0.586782	-0.514032
5	6	0	3.469399	0.920147	-0.238639
6	1	0	1.342803	0.988217	1.596524
7	1	0	0.053809	1.300266	0.417412
8	1	0	1.750245	1.601232	-1.389742
9	1	0	2.137373	2.631207	-0.029466
10	1	0	2.615251	-1.166916	1.433972
11	1	0	2.192781	-2.311551	0.148311
12	1	0	4.324172	-1.083594	-0.316884
13	1	0	3.143092	-0.772636	-1.570430
14	1	0	3.876569	1.082768	0.768035
15	1	0	4.169190	1.385005	-0.938793
16	6	0	-3.856573	0.018728	-0.200063
17	7	0	-2.749679	0.615794	0.014964
18	6	0	-2.800641	2.058773	0.244750
19	1	0	-3.818417	2.471480	0.210641
20	1	0	-2.367525	2.287868	1.225226
21	1	0	-2.194926	2.570197	-0.512247
22	1	0	-4.803127	0.581221	-0.208529

23	6	0	-3.969315	-1.451977	-0.452812
24	1	0	-4.438330	-1.633497	-1.427353
25	1	0	-2.993251	-1.942127	-0.429867
26	1	0	-4.621117	-1.916000	0.297179
27	6	0	0.316910	-0.862919	-1.066567
28	1	0	0.254511	-1.941719	-1.216676
29	1	0	-0.681917	-0.421275	-1.055797
30	1	0	0.925070	-0.420094	-1.851205
31	7	0	0.945737	-0.607746	0.281319
32	6	0	0.040901	-1.206927	1.328000
33	1	0	-0.944165	-0.745504	1.229897
34	1	0	0.464192	-1.014526	2.314506
35	1	0	-0.024802	-2.282821	1.158188

CPn_3B

SCF Done: E(RB3LYP) = -504.23438092 A.U.

Sum of electronic and thermal Free Energies= -503.951544 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.995631	1.673959	-0.333696
2	6	0	1.003748	0.910305	0.541488
3	6	0	2.424512	-1.139891	0.396981
4	6	0	3.428970	-0.399261	-0.483313
5	6	0	3.417491	1.109771	-0.202941
6	1	0	1.262441	1.023091	1.598537
7	1	0	-0.026575	1.242630	0.398991
8	1	0	1.671939	1.668019	-1.380795
9	1	0	1.962620	2.720862	-0.013807
10	1	0	2.692136	-1.037094	1.452884
11	1	0	2.370052	-2.205095	0.159212
12	1	0	4.415098	-0.826790	-0.273900
13	1	0	3.231753	-0.596631	-1.543118
14	1	0	3.795369	1.298113	0.810602
15	1	0	4.092972	1.626250	-0.890655
16	6	0	-3.771814	0.665689	-0.065573
17	7	0	-2.946553	-0.303172	-0.151946
18	6	0	-3.493333	-1.624764	-0.456008
19	1	0	-4.585012	-1.628007	-0.580160
20	1	0	-3.038818	-2.005158	-1.377871
21	1	0	-3.233903	-2.321844	0.348892
22	1	0	-4.849707	0.498018	-0.215891
23	6	0	-3.367106	2.073915	0.237815
24	1	0	-3.872351	2.426974	1.144807
25	1	0	-2.286632	2.160151	0.374859
26	1	0	-3.679598	2.741563	-0.574120
27	6	0	0.412441	-0.894882	-1.078929
28	1	0	0.440323	-1.974436	-1.234264
29	1	0	-0.620615	-0.540293	-1.077995
30	1	0	0.990688	-0.399211	-1.854485
31	7	0	1.002932	-0.595952	0.277484
32	6	0	0.130537	-1.261611	1.311860
33	1	0	-0.887639	-0.884284	1.193484
34	1	0	0.519977	-1.032549	2.304406
35	1	0	0.154374	-2.339792	1.145508

CPn_4A

SCF Done: E(RB3LYP) = -504.23259074 A.U.

Sum of electronic and thermal Free Energies= -503.949788 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.987903	1.846426	-0.332626
2	6	0	2.069920	0.911282	-0.864623
3	6	0	1.807623	-0.558788	1.139153
4	6	0	0.723944	0.367445	1.687117
5	6	0	0.917591	1.809674	1.199612
6	1	0	2.089921	0.876619	-1.956747
7	1	0	3.056584	1.226205	-0.511925
8	1	0	1.231264	2.852458	-0.690685
9	1	0	0.015227	1.588849	-0.765061
10	1	0	1.642158	-1.602188	1.419296
11	1	0	2.795410	-0.257608	1.501071
12	1	0	-0.271371	0.006384	1.405483
13	1	0	0.782969	0.313153	2.779517
14	1	0	0.095052	2.437646	1.553060
15	1	0	1.840177	2.228867	1.623099
16	6	0	-3.541131	0.078842	-0.275244
17	7	0	-2.537596	-0.632831	0.060290
18	6	0	-2.808453	-1.901592	0.732257
19	1	0	-2.388750	-2.723716	0.141202
20	1	0	-2.309872	-1.911886	1.708251
21	1	0	-3.879146	-2.096308	0.886312
22	1	0	-4.566354	-0.260417	-0.058351
23	6	0	-3.423727	1.397449	-0.973216
24	1	0	-3.958692	1.368823	-1.930135
25	1	0	-3.895551	2.186778	-0.375575
26	1	0	-2.379757	1.661773	-1.155894
27	6	0	3.112560	-1.320212	-0.812829
28	1	0	3.010223	-2.346347	-0.457613
29	1	0	3.177865	-1.310452	-1.901645
30	1	0	4.006331	-0.866868	-0.383295
31	7	0	1.902484	-0.532420	-0.388092
32	6	0	0.680142	-1.167631	-1.009046
33	1	0	0.769045	-1.091690	-2.093816
34	1	0	-0.236599	-0.682273	-0.669270
35	1	0	0.661413	-2.218415	-0.715995

CPn_4B

SCF Done: E(RB3LYP) = -504.23283516 A.U.

Sum of electronic and thermal Free Energies= -503.950175 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.197601	1.822580	-0.225110
2	6	0	-2.173107	0.788725	-0.781281
3	6	0	-1.688118	-0.729870	1.142548
4	6	0	-0.708290	0.292009	1.714900
5	6	0	-1.083049	1.721886	1.302015
6	1	0	-3.181208	0.964645	-0.394327
7	1	0	-2.215756	0.801799	-1.873214
8	1	0	-0.212879	1.708877	-0.689996
9	1	0	-1.572323	2.806923	-0.525654
10	1	0	-2.695168	-0.563392	1.536770
11	1	0	-1.395264	-1.758185	1.369022
12	1	0	-0.734760	0.181083	2.804280
13	1	0	0.315729	0.065003	1.399561
14	1	0	-2.037344	2.006914	1.764816
15	1	0	-0.332153	2.426745	1.669698
16	6	0	3.510896	-0.428835	0.031174
17	7	0	2.535214	0.273614	-0.393491
18	6	0	2.855717	1.504458	-1.112433
19	1	0	3.935380	1.681163	-1.218271
20	1	0	2.409678	1.468952	-2.112802
21	1	0	2.414118	2.358412	-0.586500
22	1	0	4.550323	-0.109105	-0.143178
23	6	0	3.339156	-1.711997	0.783070

24	1	0	3.835538	-2.532910	0.251612
25	1	0	3.818722	-1.642563	1.766885
26	1	0	2.283444	-1.959203	0.917604
27	6	0	-0.549094	-1.097225	-1.053865
28	1	0	-0.381638	-2.143444	-0.793261
29	1	0	-0.683226	-1.006495	-2.132945
30	1	0	0.305374	-0.500003	-0.729409
31	7	0	-1.822825	-0.645133	-0.379553
32	6	0	-2.940208	-1.553025	-0.817917
33	1	0	-3.036834	-1.497914	-1.903053
34	1	0	-3.869865	-1.233684	-0.345883
35	1	0	-2.704425	-2.575219	-0.519052

CPn_5

SCF Done: E(RB3LYP) = -504.22592385 A.U.

Sum of electronic and thermal Free Energies= -503.943303 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.612343	0.734913	1.464686
2	6	0	-1.371818	-0.564629	1.228899
3	6	0	-1.687665	0.475111	-1.055051
4	6	0	-2.328444	1.578984	-0.221453
5	6	0	-1.436057	1.952353	0.985149
6	1	0	-0.856224	-1.437596	1.634284
7	1	0	-2.368572	-0.519847	1.674498
8	1	0	-0.399987	0.805522	2.536018
9	1	0	0.360334	0.689347	0.961879
10	1	0	-0.670899	0.751337	-1.341053
11	1	0	-2.250447	0.245309	-1.962457
12	1	0	-2.487438	2.441205	-0.876091
13	1	0	-3.327825	1.269702	0.106722
14	1	0	-0.755204	2.764150	0.712274
15	1	0	-2.064332	2.331763	1.796734
16	6	0	3.548167	-0.094783	0.154994
17	7	0	2.520264	0.213861	-0.533974
18	6	0	2.721239	1.078019	-1.694866
19	1	0	2.371525	0.563248	-2.596944
20	1	0	2.119608	1.987137	-1.581641
21	1	0	3.769519	1.371678	-1.845825
22	1	0	4.544236	0.283731	-0.123219
23	6	0	3.495716	-0.972952	1.365982
24	1	0	4.142085	-1.848012	1.227979
25	1	0	3.880864	-0.436148	2.241359
26	1	0	2.477093	-1.309864	1.572117
27	6	0	-2.824678	-1.657859	-0.451286
28	1	0	-2.901917	-1.965525	-1.494834
29	1	0	-2.768073	-2.538262	0.190639
30	1	0	-3.690260	-1.055115	-0.175388
31	7	0	-1.572910	-0.843248	-0.271212
32	6	0	-0.398772	-1.623422	-0.809973
33	1	0	-0.382793	-2.603754	-0.330944
34	1	0	0.526460	-1.075261	-0.605543
35	1	0	-0.531298	-1.743446	-1.886749

CPn_6

SCF Done: E(RB3LYP) = -504.22429847 A.U.

Sum of electronic and thermal Free Energies= -503.941885 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.300405	-0.776217	-0.564294
2	6	0	2.281915	-1.192801	0.502615
3	6	0	1.099751	1.031160	0.441014
4	6	0	2.548880	1.499075	0.272121
5	6	0	3.272319	0.747476	-0.850700
6	1	0	2.091122	-2.268271	0.484311
7	1	0	2.627258	-0.930930	1.505388
8	1	0	4.280822	-1.078525	-0.182291
9	1	0	3.147355	-1.348756	-1.483607
10	1	0	0.450576	1.450889	-0.328493
11	1	0	0.702980	1.327636	1.412851
12	1	0	2.518300	2.573755	0.066221
13	1	0	3.094914	1.385280	1.215430
14	1	0	2.771281	0.947956	-1.805152
15	1	0	4.290056	1.130428	-0.959416
16	6	0	-3.886665	-0.014818	-0.230157
17	7	0	-2.783504	0.604094	-0.063278
18	6	0	-2.839613	2.061276	0.036870
19	1	0	-2.412500	2.377984	0.995159
20	1	0	-2.229509	2.505435	-0.758036
21	1	0	-3.858282	2.465976	-0.040618
22	1	0	-4.835720	0.539966	-0.294205
23	6	0	-3.990234	-1.502987	-0.350922
24	1	0	-4.646772	-1.901734	0.431758
25	1	0	-4.449025	-1.773780	-1.309513
26	1	0	-3.011860	-1.983159	-0.275145
27	6	0	0.002268	-0.975078	1.430210
28	1	0	-0.958797	-0.474030	1.294022
29	1	0	-0.122616	-2.055640	1.341708
30	1	0	0.440965	-0.732636	2.398818
31	7	0	0.933313	-0.505377	0.340471
32	6	0	0.308171	-0.872057	-0.984883
33	1	0	0.266719	-1.960098	-1.060030
34	1	0	0.910436	-0.468113	-1.796208
35	1	0	-0.699542	-0.450827	-1.004542

CPn_7

SCF Done: E(RB3LYP) = -504.22384606 A.U.

Sum of electronic and thermal Free Energies= -503.940964 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.198353	1.833039	0.006009
2	6	0	-1.174315	0.793208	1.130432
3	6	0	-1.047969	-0.731256	-0.872466
4	6	0	-2.000396	0.138087	-1.700703
5	6	0	-2.264906	1.519441	-1.049108
6	1	0	-0.231543	0.833652	1.676343
7	1	0	-1.988975	0.954458	1.839610
8	1	0	-1.383006	2.806707	0.471232
9	1	0	-0.210280	1.894896	-0.462667
10	1	0	-0.007403	-0.415974	-0.976686
11	1	0	-1.114888	-1.785533	-1.152065
12	1	0	-1.523072	0.260639	-2.678349
13	1	0	-2.940400	-0.388842	-1.890057
14	1	0	-2.275698	2.301864	-1.811918
15	1	0	-3.257439	1.539749	-0.583070
16	6	0	3.450981	0.408037	0.030975
17	7	0	2.527615	-0.395352	-0.328178
18	6	0	2.902579	-1.495649	-1.215030
19	1	0	2.646833	-2.450138	-0.741230
20	1	0	2.326520	-1.428055	-2.144936
21	1	0	3.971648	-1.508375	-1.468538
22	1	0	4.484879	0.266754	-0.320689
23	6	0	3.223248	1.578598	0.935311
24	1	0	3.845399	1.490803	1.834182
25	1	0	3.525016	2.507786	0.437194

26	1	0	2.174697	1.657003	1.232488
27	6	0	-2.717751	-1.170756	0.920585
28	1	0	-2.819113	-2.176371	0.509609
29	1	0	-2.858185	-1.197768	2.001813
30	1	0	-3.456053	-0.509766	0.471081
31	7	0	-1.331340	-0.662653	0.626496
32	6	0	-0.334024	-1.541293	1.340175
33	1	0	-0.488111	-1.442552	2.415943
34	1	0	0.670260	-1.216833	1.057424
35	1	0	-0.499583	-2.576793	1.037971

CPn_8

SCF Done: E(RB3LYP) = -504.22329779 A.U.

Sum of electronic and thermal Free Energies= -503.941600 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.519468	1.365287	-0.594649
2	6	0	1.436274	0.435215	-1.155313
3	6	0	0.849267	-0.507927	1.100679
4	6	0	1.174794	0.934008	1.511011
5	6	0	2.515454	1.422953	0.953873
6	1	0	0.452270	0.907576	-1.136381
7	1	0	1.647973	0.137810	-2.185030
8	1	0	3.505266	1.077029	-0.971301
9	1	0	2.316008	2.355421	-1.015245
10	1	0	-0.226907	-0.679569	1.146729
11	1	0	1.357528	-1.234379	1.738120
12	1	0	0.367501	1.598067	1.183338
13	1	0	1.171671	0.967260	2.605064
14	1	0	2.708425	2.443947	1.292606
15	1	0	3.329031	0.812994	1.363813
16	6	0	-3.490067	0.663311	-0.170751
17	7	0	-2.717534	-0.290835	0.174200
18	6	0	-3.320722	-1.426695	0.869046
19	1	0	-3.132818	-2.344123	0.299835
20	1	0	-2.847611	-1.547723	1.850238
21	1	0	-4.404915	-1.324365	1.015846
22	1	0	-4.567592	0.621905	0.052884
23	6	0	-3.019192	1.888168	-0.890650
24	1	0	-3.535882	1.985487	-1.853084
25	1	0	-3.263845	2.787183	-0.312328
26	1	0	-1.940978	1.857964	-1.066215
27	6	0	2.567931	-1.627077	-0.355522
28	1	0	2.403337	-2.575272	0.157090
29	1	0	2.862332	-1.812868	-1.389655
30	1	0	3.344557	-1.064487	0.157432
31	7	0	1.278644	-0.848194	-0.349334
32	6	0	0.207748	-1.697145	-0.988027
33	1	0	0.509296	-1.935745	-2.009238
34	1	0	-0.734622	-1.145157	-0.968122
35	1	0	0.106473	-2.616339	-0.408641

TSs_1A

SCF Done: E(RB3LYP) = -1562.19968916 A.U.

Sum of electronic and thermal Free Energies= -1561.758599 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.821609	1.557902	-0.771381
2	6	0	-2.459858	0.562910	0.008383
3	6	0	-2.111537	0.303421	1.369731
4	1	0	-2.025211	1.574291	-1.837689
5	1	0	-2.751910	-0.422731	1.866087
6	8	0	-3.270455	-0.248976	-0.679819
7	14	0	-4.717776	-1.114808	-0.300866
8	6	0	-4.285780	-2.741141	0.538814
9	1	0	-3.592470	-3.332147	-0.069564
10	1	0	-3.841981	-2.606431	1.530737
11	1	0	-5.196401	-3.338325	0.669106
12	6	0	-5.471365	-1.406842	-1.989262
13	1	0	-6.407412	-1.970663	-1.904699
14	1	0	-5.693403	-0.460444	-2.493194
15	1	0	-4.793064	-1.980027	-2.630381
16	6	0	-5.789844	-0.022573	0.788565
17	1	0	-5.984981	0.944219	0.311989
18	1	0	-6.758357	-0.507101	0.960050
19	1	0	-5.340644	0.166388	1.768955
20	8	0	-0.275790	3.295800	-1.065750
21	6	0	0.414743	4.387732	-0.435545
22	1	0	0.939342	4.915358	-1.231520
23	1	0	-0.299547	5.064223	0.044029
24	1	0	1.130756	4.013649	0.304185
25	6	0	-0.418059	-0.404705	1.454307
26	7	0	0.565404	0.534178	1.304183
27	6	0	0.756696	1.353282	2.488705
28	1	0	-0.099682	2.021976	2.719173
29	1	0	0.910752	0.756663	3.405224
30	1	0	1.630565	2.005983	2.365998
31	1	0	-0.546573	-0.778755	2.484759
32	6	0	-0.374692	-1.552962	0.453833
33	1	0	0.533873	-2.144568	0.613065
34	1	0	-1.232320	-2.222093	0.563780
35	1	0	-0.363929	-1.180671	-0.575763
36	6	0	-0.928675	2.454740	-0.251308
37	1	0	-0.770460	2.593159	0.810948
38	1	0	-1.972732	1.188392	1.989868
39	6	0	5.011050	-1.111708	1.345817
40	6	0	3.923675	-0.137708	0.880555
41	6	0	4.745779	-0.795433	-1.717542
42	6	0	5.765317	-1.717033	-1.034401
43	6	0	6.186951	-1.230000	0.361735
44	1	0	3.061669	-0.077711	1.549831
45	1	0	4.320262	0.868032	0.704954
46	1	0	5.370169	-0.747580	2.314891
47	1	0	4.568851	-2.098228	1.532571
48	1	0	4.444310	-1.167311	-2.700266
49	1	0	5.122921	0.227207	-1.821450
50	1	0	5.361249	-2.735485	-0.976966
51	1	0	6.639732	-1.769212	-1.692550
52	1	0	6.927832	-1.923809	0.770724
53	1	0	6.689175	-0.257122	0.273127
54	16	0	3.206657	-0.720538	-0.709317
55	6	0	2.316743	0.739079	-1.319183
56	1	0	1.875013	0.479450	-2.283082
57	1	0	1.537465	0.908092	-0.553661
58	1	0	3.004420	1.581634	-1.417712

TSs_1B

SCF Done: E(RB3LYP) = -1562.19970292 A.U.

Sum of electronic and thermal Free Energies= -1561.757375 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.981609	-0.099189	-0.503354
2	6	0	4.805022	0.356531	-1.375628

3	6	0	3.328241	-1.622794	-0.069806
4	6	0	4.624702	-1.917918	0.691602
5	6	0	5.897642	-1.580218	-0.101138
6	1	0	4.876653	1.413963	-1.644202
7	1	0	4.723096	-0.238073	-2.291300
8	1	0	6.897239	0.082460	-1.076998
9	1	0	6.046107	0.534559	0.390187
10	1	0	2.423992	-1.808568	0.514147
11	1	0	3.281593	-2.153880	-1.026565
12	1	0	4.619072	-1.384128	1.649995
13	1	0	4.608728	-2.986095	0.936050
14	1	0	6.774582	-1.837055	0.501097
15	1	0	5.945343	-2.206673	-1.002081
16	16	0	3.221508	0.176812	-0.442915
17	6	0	1.984381	0.296018	-1.766951
18	1	0	1.025029	0.156282	-1.269095
19	1	0	2.049360	1.303396	-2.182846
20	1	0	2.175641	-0.458740	-2.532002
21	6	0	-1.518706	1.603033	-0.375214
22	6	0	-2.338579	0.579990	0.161006
23	6	0	-2.035551	-0.077984	1.391530
24	1	0	-1.713376	1.931102	-1.391786
25	1	0	-2.791781	-0.785237	1.724627
26	8	0	-3.293851	0.136626	-0.664378
27	14	0	-4.866668	-0.542869	-0.427083
28	6	0	-4.713737	-2.377117	-0.040125
29	1	0	-4.148146	-2.902921	-0.817033
30	1	0	-4.233227	-2.571383	0.924495
31	1	0	-5.712709	-2.827985	-0.001692
32	6	0	-5.684121	-0.264394	-2.087486
33	1	0	-6.700153	-0.675219	-2.093774
34	1	0	-5.751908	0.803215	-2.321212
35	1	0	-5.122223	-0.751163	-2.891788
36	6	0	-5.713546	0.400814	0.959268
37	1	0	-5.730540	1.476584	0.753475
38	1	0	-6.753649	0.066467	1.052166
39	1	0	-5.233412	0.248198	1.931354
40	8	0	0.352225	3.020652	-0.290645
41	6	0	1.216319	3.777059	0.575163
42	1	0	1.828917	4.401101	-0.075201
43	1	0	0.626336	4.414409	1.240981
44	1	0	1.850933	3.105670	1.163439
45	6	0	-0.489147	-1.067616	1.195973
46	7	0	0.641717	-0.297429	1.195131
47	6	0	1.025144	0.136654	2.529684
48	1	0	0.292055	0.817378	3.010544
49	1	0	1.143524	-0.704250	3.234533
50	1	0	1.977882	0.679081	2.496778
51	1	0	-0.656714	-1.642221	2.122682
52	6	0	-0.693536	-1.943589	-0.034266
53	1	0	0.109239	-2.687252	-0.098419
54	1	0	-1.642252	-2.484916	0.008957
55	1	0	-0.685899	-1.354596	-0.956752
56	6	0	-0.466207	2.143670	0.313171
57	1	0	-0.302291	1.986843	1.371214
58	1	0	-1.726428	0.576898	2.205525

TSs_2A

SCF Done: E(RB3LYP) = -1562.19915128 A.U.

Sum of electronic and thermal Free Energies= -1561.756298 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.963940	-1.361502	1.060845
2	6	0	4.156806	-0.087532	0.788639
3	6	0	3.280635	-1.401804	-1.529507
4	6	0	4.162458	-2.565244	-1.060551
5	6	0	4.324844	-2.627291	0.467105
6	1	0	4.646018	0.803275	1.191502
7	1	0	3.120256	-0.139352	1.147894
8	1	0	5.038757	-1.458290	2.149824
9	1	0	5.990257	-1.243995	0.690436
10	1	0	3.194687	-1.359736	-2.618467
11	1	0	2.283516	-1.428752	-1.082370
12	1	0	5.144171	-2.507620	-1.547316
13	1	0	3.691745	-3.485383	-1.424515
14	1	0	4.943513	-3.492924	0.723283
15	1	0	3.344805	-2.793350	0.932494
16	16	0	4.044125	0.198549	-1.031603
17	6	0	2.657175	1.374107	-1.169464
18	1	0	2.311663	1.345926	-2.205145
19	1	0	3.066797	2.363508	-0.956122
20	1	0	1.868278	1.090852	-0.448949
21	6	0	-1.636368	1.631703	-0.698889
22	6	0	-2.263430	0.606165	0.049702
23	6	0	-1.892192	0.290653	1.394651
24	1	0	-1.861721	1.697258	-1.758875
25	1	0	-2.533706	-0.447331	1.871817
26	8	0	-3.089655	-0.174472	-0.654429
27	14	0	-4.544702	-1.035387	-0.287510
28	6	0	-4.125303	-2.686568	0.509701
29	1	0	-3.444743	-3.272432	-0.117773
30	1	0	-3.672920	-2.580906	1.501273
31	1	0	-5.042606	-3.274940	0.632967
32	6	0	-5.311620	-1.276529	-1.977538
33	1	0	-6.250898	-1.836099	-1.901268
34	1	0	-5.530767	-0.315374	-2.454023
35	1	0	-4.642088	-1.836722	-2.638992
36	6	0	-5.595403	0.041357	0.837015
37	1	0	-5.785120	1.021088	0.385404
38	1	0	-6.567174	-0.437615	1.005635
39	1	0	-5.135987	0.202115	1.817747
40	8	0	-0.100701	3.389157	-0.937774
41	6	0	0.538588	4.490123	-0.269216
42	1	0	1.084565	5.037606	-1.037033
43	1	0	-0.211112	5.145716	0.184272
44	1	0	1.229359	4.126252	0.499348
45	6	0	-0.216017	-0.433351	1.427031
46	7	0	0.780791	0.495439	1.289580
47	6	0	1.006127	1.268973	2.498757
48	1	0	0.158075	1.929653	2.777192
49	1	0	1.184950	0.638463	3.387380
50	1	0	1.878730	1.923634	2.377016
51	1	0	-0.327122	-0.843263	2.445951
52	6	0	-0.202584	-1.548247	0.388425
53	1	0	0.688252	-2.170803	0.532770
54	1	0	-1.076961	-2.199147	0.472188
55	1	0	-0.179853	-1.136855	-0.626331
56	6	0	-0.736242	2.506000	-0.154082
57	1	0	-0.555837	2.591423	0.910362
58	1	0	-1.741127	1.151122	2.046030

TSs_2B

SCF Done: E(RB3LYP) = -1562.19930801 A.U.

Sum of electronic and thermal Free Energies= -1561.7566 A.U.

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

1	6	0	-1.566104	1.651803	-0.447140
2	6	0	-2.291608	0.598596	0.162119
3	6	0	-1.879042	-0.019162	1.384256
4	1	0	-1.849728	1.948548	-1.452237
5	1	0	-2.588637	-0.742981	1.779890
6	8	0	-3.277606	0.095432	-0.586386
7	14	0	-4.809942	-0.632503	-0.244208
8	6	0	-4.570234	-2.453394	0.157122
9	1	0	-4.025690	-2.970591	-0.640265
10	1	0	-4.036548	-2.616456	1.099178
11	1	0	-5.549122	-2.938943	0.251350
12	6	0	-5.734452	-0.404671	-1.855027
13	1	0	-6.737965	-0.840843	-1.792568
14	1	0	-5.844425	0.656710	-2.100755
15	1	0	-5.209970	-0.890742	-2.684600
16	6	0	-5.598469	0.306390	1.178964
17	1	0	-5.677121	1.375336	0.952986
18	1	0	-6.613569	-0.069278	1.353748
19	1	0	-5.043579	0.197119	2.116398
20	8	0	0.203487	3.190512	-0.515590
21	6	0	1.044432	4.048411	0.273383
22	1	0	1.615483	4.650052	-0.433289
23	1	0	0.434769	4.704093	0.902730
24	1	0	1.721664	3.456039	0.898543
25	6	0	-0.328729	-0.953115	1.120272
26	7	0	0.782534	-0.152212	1.064678
27	6	0	1.191022	0.326376	2.373924
28	1	0	0.457621	1.007035	2.855563
29	1	0	1.349138	-0.489316	3.101161
30	1	0	2.130008	0.891116	2.304425
31	1	0	-0.429147	-1.534949	2.052884
32	6	0	-0.556134	-1.837713	-0.100145
33	1	0	0.245749	-2.580949	-0.174429
34	1	0	-1.502781	-2.380332	-0.036659
35	1	0	-0.563718	-1.248666	-1.022497
36	6	0	-0.507964	2.273439	0.157026
37	1	0	-0.248492	2.133486	1.199082
38	1	0	-1.554716	0.670809	2.163012
39	6	0	4.578026	-2.343543	0.104690
40	6	0	3.310714	-1.843548	-0.597383
41	6	0	4.366983	0.716423	-0.218955
42	6	0	5.546066	0.007316	0.458188
43	6	0	5.157136	-1.331477	1.106583
44	1	0	2.924519	-2.567477	-1.319785
45	1	0	2.515571	-1.542216	0.099279
46	1	0	4.304110	-3.267521	0.626286
47	1	0	5.337084	-2.621865	-0.637443
48	1	0	4.663902	1.657988	-0.688153
49	1	0	3.534410	0.888558	0.468890
50	1	0	6.356332	-0.140101	-0.266908
51	1	0	5.934569	0.693095	1.219456
52	1	0	6.042504	-1.765677	1.581261
53	1	0	4.427372	-1.152508	1.906270
54	16	0	3.705561	-0.333332	-1.580461
55	6	0	2.062492	0.395025	-1.883387
56	1	0	2.222616	1.403988	-2.269234
57	1	0	1.583688	-0.214923	-2.652442
58	1	0	1.494703	0.385711	-0.938718

TSs_3A

SCF Done: E(RB3LYP) = -1562.19878194 A.U.

Sum of electronic and thermal Free Energies= -1561.757439 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.566778	1.512058	-0.797759
2	6	0	-2.342387	0.602990	-0.036744
3	6	0	-2.124326	0.380995	1.357158
4	1	0	-1.680674	1.497079	-1.877338
5	1	0	-2.848770	-0.280353	1.827534
6	8	0	-3.156146	-0.176457	-0.758332
7	14	0	-4.683413	-0.928900	-0.457119
8	6	0	-4.428750	-2.535477	0.487165
9	1	0	-3.720283	-3.193586	-0.027582
10	1	0	-4.071050	-2.379016	1.510207
11	1	0	-5.382419	-3.072750	0.555291
12	6	0	-5.324028	-1.255806	-2.185258
13	1	0	-6.296667	-1.759655	-2.148944
14	1	0	-5.449329	-0.323053	-2.744866
15	1	0	-4.636502	-1.897045	-2.747202
16	6	0	-5.758973	0.282734	0.493701
17	1	0	-5.856913	1.232320	-0.043466
18	1	0	-6.766304	-0.132406	0.616590
19	1	0	-5.369193	0.496848	1.494184
20	8	0	0.134500	3.113986	-1.016366
21	6	0	0.826804	4.194284	-0.366687
22	1	0	1.466170	4.645911	-1.124711
23	1	0	0.112278	4.938098	-0.000778
24	1	0	1.434091	3.817851	0.463302
25	6	0	-0.488086	-0.435562	1.607987
26	7	0	0.565811	0.425780	1.478913
27	6	0	0.740773	1.286983	2.637952
28	1	0	-0.087187	2.010331	2.792128
29	1	0	0.811947	0.723091	3.584135
30	1	0	1.656890	1.882340	2.537151
31	1	0	-0.718534	-0.736610	2.644202
32	6	0	-0.462330	-1.640727	0.676049
33	1	0	0.390452	-2.281851	0.927815
34	1	0	-1.369801	-2.243322	0.766908
35	1	0	-0.362512	-1.333219	-0.369753
36	6	0	-0.651431	2.358757	-0.234427
37	1	0	-0.577711	2.531994	0.831394
38	1	0	-1.970089	1.279581	1.953306
39	6	0	5.237334	-1.600857	-1.442909
40	6	0	5.252865	-0.096745	-1.162863
41	6	0	3.637241	-0.783720	1.107063
42	6	0	3.799151	-2.210797	0.583823
43	6	0	5.111598	-2.459326	-0.174561
44	1	0	6.121335	0.193902	-0.562523
45	1	0	5.260187	0.507574	-2.074562
46	1	0	4.433673	-1.846342	-2.147402
47	1	0	6.175321	-1.830588	-1.961627
48	1	0	4.396330	-0.527345	1.853071
49	1	0	2.635123	-0.577755	1.511522
50	1	0	3.744203	-2.866957	1.460388
51	1	0	2.942338	-2.476594	-0.046516
52	1	0	5.966394	-2.266832	0.488024
53	1	0	5.169488	-3.515602	-0.454483
54	16	0	3.818397	0.523454	-0.182287
55	6	0	2.357114	0.268281	-1.233677
56	1	0	1.512051	0.392670	-0.538161
57	1	0	2.361852	1.052794	-1.992201
58	1	0	2.364977	-0.721230	-1.689681

TSs_3B

SCF Done: E(RB3LYP) = -1562.19895098 A.U.

Sum of electronic and thermal Free Energies= -1561.756617 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.808793	-0.528740	-1.065717
2	6	0	4.710125	-1.415801	-1.654507
3	6	0	3.537661	-1.221951	0.952812
4	6	0	4.761448	-0.359941	1.264040
5	6	0	6.009688	-0.723422	0.445053
6	1	0	4.952383	-2.479108	-1.554860
7	1	0	4.519375	-1.215106	-2.712663
8	1	0	5.603636	0.525484	-1.287218
9	1	0	6.731601	-0.776597	-1.602889
10	1	0	3.699184	-2.274183	1.208460
11	1	0	2.616009	-0.865837	1.433175
12	1	0	4.965357	-0.488661	2.333364
13	1	0	4.515981	0.699966	1.128502
14	1	0	6.296418	-1.764186	0.648333
15	1	0	6.848225	-0.102374	0.774676
16	16	0	3.066545	-1.263062	-0.829658
17	6	0	2.514266	0.440327	-1.145703
18	1	0	1.716547	0.606407	-0.397340
19	1	0	2.117006	0.467557	-2.161701
20	1	0	3.335233	1.147600	-1.029358
21	6	0	-1.609421	1.509963	-0.821146
22	6	0	-2.375063	0.621948	-0.025325
23	6	0	-2.107819	0.396265	1.359346
24	1	0	-1.772454	1.497324	-1.894417
25	1	0	-2.834677	-0.240437	1.859171
26	8	0	-3.239113	-0.135937	-0.709896
27	14	0	-4.777291	-0.835757	-0.340650
28	6	0	-4.539944	-2.437165	0.616736
29	1	0	-3.876627	-3.127219	0.084015
30	1	0	-4.135744	-2.279930	1.622138
31	1	0	-5.508320	-2.939125	0.731209
32	6	0	-5.492593	-1.164825	-2.038721
33	1	0	-6.477525	-1.638944	-1.958964
34	1	0	-5.611570	-0.235892	-2.605973
35	1	0	-4.845992	-1.833446	-2.617093
36	6	0	-5.774764	0.424137	0.632292
37	1	0	-5.859831	1.369634	0.085789
38	1	0	-6.790493	0.045979	0.797866
39	1	0	-5.340776	0.637416	1.614619
40	8	0	0.114443	3.071128	-1.123410
41	6	0	0.865981	4.133706	-0.512734
42	1	0	1.481977	4.563453	-1.302145
43	1	0	0.190630	4.898976	-0.117727
44	1	0	1.500374	3.743770	0.290562
45	6	0	-0.493387	-0.470958	1.550825
46	7	0	0.583711	0.357715	1.401450
47	6	0	0.815560	1.209774	2.555550
48	1	0	0.020190	1.966084	2.724459
49	1	0	0.882866	0.644573	3.501468
50	1	0	1.752573	1.767745	2.435174
51	1	0	-0.702395	-0.778804	2.589782
52	6	0	-0.525255	-1.663942	0.603717
53	1	0	0.301249	-2.344504	0.839855
54	1	0	-1.455291	-2.231550	0.691986
55	1	0	-0.418468	-1.343773	-0.437792
56	6	0	-0.650024	2.335572	-0.303012
57	1	0	-0.515047	2.500641	0.758504
58	1	0	-1.904369	1.291439	1.945923

TSs_4

SCF Done: E(RB3LYP) = -1562.19627950 A.U.

Sum of electronic and thermal Free Energies= -1561.754772 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.438333	0.825818	-0.611514
2	6	0	-3.046826	0.340285	-1.019551
3	6	0	-3.520304	-1.782458	0.775562
4	6	0	-4.871000	-1.110235	1.025932
5	6	0	-4.846478	0.412180	0.812618
6	1	0	-2.779563	0.604070	-2.046565
7	1	0	-2.246745	0.672945	-0.341963
8	1	0	-4.418168	1.919631	-0.685143
9	1	0	-5.192503	0.495138	-1.336350
10	1	0	-3.551304	-2.869490	0.891286
11	1	0	-2.721554	-1.371072	1.405905
12	1	0	-5.652946	-1.571593	0.410311
13	1	0	-5.138932	-1.333037	2.065404
14	1	0	-5.839507	0.817615	1.030415
15	1	0	-4.155859	0.864870	1.533978
16	16	0	-2.826913	-1.483680	-0.906611
17	6	0	-4.079970	-2.171685	-2.038087
18	1	0	-4.063053	-3.256646	-1.916995
19	1	0	-5.076316	-1.780337	-1.837196
20	1	0	-3.767262	-1.918498	-3.053117
21	6	0	1.352562	1.470554	-0.842538
22	6	0	2.171715	0.656954	-0.023203
23	6	0	1.895918	0.432304	1.362686
24	1	0	1.529847	1.456459	-1.913505
25	1	0	2.666169	-0.131964	1.884358
26	8	0	3.105570	-0.040158	-0.679597
27	14	0	4.689133	-0.606422	-0.275078
28	6	0	4.566723	-2.186350	0.737794
29	1	0	3.964587	-2.944731	0.225798
30	1	0	4.140120	-2.023991	1.733070
31	1	0	5.569696	-2.606907	0.879141
32	6	0	5.443777	-0.936537	-1.955743
33	1	0	6.461588	-1.329923	-1.853278
34	1	0	5.495896	-0.020668	-2.553514
35	1	0	4.856138	-1.672265	-2.515200
36	6	0	5.575833	0.760088	0.660321
37	1	0	5.597485	1.688514	0.079482
38	1	0	6.614507	0.465927	0.851985
39	1	0	5.113182	0.976162	1.628915
40	8	0	-0.477634	2.899612	-1.184376
41	6	0	-1.259322	3.956796	-0.603523
42	1	0	-1.908569	4.327833	-1.396203
43	1	0	-0.607903	4.764933	-0.256667
44	1	0	-1.860024	3.579115	0.231309
45	6	0	0.369689	-0.548737	1.544245
46	7	0	-0.774752	0.184481	1.361417
47	6	0	-1.081582	1.030621	2.502596
48	1	0	-0.339202	1.837706	2.679897
49	1	0	-1.132271	0.471558	3.453546
50	1	0	-2.048668	1.529957	2.362016
51	1	0	0.575979	-0.820867	2.594155
52	6	0	0.516734	-1.758109	0.629369
53	1	0	-0.252714	-2.500624	0.871081
54	1	0	1.489778	-2.242421	0.747098
55	1	0	0.398385	-1.473158	-0.420495
56	6	0	0.328833	2.230129	-0.345797
57	1	0	0.173619	2.404764	0.711454
58	1	0	1.620798	1.323063	1.927310

TSn_1A

SCF Done: E(RB3LYP) = -1258.69332489 A.U.

Sum of electronic and thermal Free Energies= -1258.202279 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.561328	1.599738	-0.697373
2	6	0	-2.291551	0.630801	0.029848
3	6	0	-2.003722	0.318123	1.395239
4	1	0	-1.713587	1.654574	-1.770857
5	1	0	-2.699570	-0.382292	1.852488
6	8	0	-3.127057	-0.113835	-0.705297
7	14	0	-4.634519	-0.895372	-0.385180
8	6	0	-4.331103	-2.548722	0.459947
9	1	0	-3.653184	-3.178548	-0.126440
10	1	0	-3.916651	-2.444770	1.468130
11	1	0	-5.280269	-3.090150	0.553261
12	6	0	-5.343405	-1.136883	-2.100686
13	1	0	-6.310328	-1.650544	-2.051550
14	1	0	-5.497549	-0.177321	-2.605023
15	1	0	-4.675036	-1.741994	-2.722620
16	6	0	-5.678435	0.252525	0.673932
17	1	0	-5.808655	1.227779	0.192465
18	1	0	-6.675510	-0.179573	0.819682
19	1	0	-5.245523	0.418580	1.665835
20	8	0	0.112491	3.238185	-0.867593
21	6	0	0.770781	4.313638	-0.177866
22	1	0	1.403613	4.807492	-0.914998
23	1	0	0.034403	5.026183	0.206673
24	1	0	1.380766	3.927258	0.646038
25	6	0	-0.358266	-0.478855	1.508505
26	7	0	0.679134	0.404900	1.379819
27	6	0	0.913352	1.178367	2.587869
28	1	0	0.078901	1.859150	2.859103
29	1	0	1.071752	0.545328	3.478206
30	1	0	1.802591	1.811107	2.470552
31	1	0	-0.522589	-0.852930	2.533621
32	6	0	-0.362921	-1.623229	0.502424
33	1	0	0.496444	-2.277825	0.689544
34	1	0	-1.266540	-2.233731	0.580481
35	1	0	-0.295447	-1.244474	-0.522828
36	6	0	-0.636295	2.420397	-0.110103
37	1	0	-0.536053	2.534580	0.961562
38	1	0	-1.838206	1.178702	2.043022
39	6	0	4.925676	-1.302327	1.054041
40	6	0	4.081116	-0.086956	0.678819
41	6	0	3.126331	-1.316894	-1.266028
42	6	0	3.950801	-2.552991	-0.910608
43	6	0	4.267595	-2.609275	0.590454
44	1	0	3.096919	-0.118669	1.159929
45	1	0	4.573188	0.853771	0.939948
46	1	0	5.940944	-1.216443	0.647977
47	1	0	5.034551	-1.290171	2.143779
48	1	0	2.157713	-1.337913	-0.762525
49	1	0	2.959057	-1.228207	-2.342721
50	1	0	3.364204	-3.425933	-1.216509
51	1	0	4.873893	-2.588737	-1.501049
52	1	0	3.340006	-2.769563	1.154293
53	1	0	4.921179	-3.459670	0.805911
54	6	0	5.015826	0.276963	-1.617638
55	1	0	4.740592	0.361734	-2.669878
56	1	0	5.442633	1.219065	-1.271396
57	1	0	5.742878	-0.521817	-1.492184
58	7	0	3.776354	-0.008953	-0.819264
59	6	0	2.783257	1.108010	-1.034858
60	1	0	3.270027	2.049782	-0.774829
61	1	0	1.916859	0.928374	-0.383130
62	1	0	2.496703	1.122021	-2.087715

TSn_1B

SCF Done: E(RB3LYP) = -1258.69338638 A.U.

Sum of electronic and thermal Free Energies= -1258.204199 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.547552	1.597025	0.559191
2	6	0	2.319520	0.616196	-0.106866
3	6	0	1.975980	0.114669	-1.401081
4	1	0	1.767344	1.794896	1.603837
5	1	0	2.704776	-0.574737	-1.822503
6	8	0	3.270425	0.046931	0.643074
7	14	0	4.820736	-0.641029	0.311732
8	6	0	4.615281	-2.422923	-0.252237
9	1	0	4.036168	-3.005905	0.472172
10	1	0	4.128090	-2.508858	-1.229047
11	1	0	5.600828	-2.896299	-0.338729
12	6	0	5.668417	-0.553158	1.978252
13	1	0	6.677639	-0.977152	1.924335
14	1	0	5.757060	0.482102	2.323696
15	1	0	5.109922	-1.115026	2.734595
16	6	0	5.672831	0.416615	-0.986396
17	1	0	5.720312	1.465563	-0.674250
18	1	0	6.702627	0.068477	-1.129752
19	1	0	5.174930	0.373949	-1.960557
20	8	0	-0.259498	3.088410	0.681397
21	6	0	-1.086989	3.994842	-0.064912
22	1	0	-1.685041	4.536380	0.667705
23	1	0	-0.468556	4.702462	-0.625974
24	1	0	-1.738981	3.444011	-0.751794
25	6	0	0.408283	-0.828716	-1.300146
26	7	0	-0.698731	-0.025469	-1.219341
27	6	0	-1.050863	0.566696	-2.498722
28	1	0	-0.299892	1.288130	-2.885629
29	1	0	-1.172062	-0.182471	-3.300446
30	1	0	-1.994981	1.121479	-2.421843
31	1	0	0.550053	-1.319479	-2.278452
32	6	0	0.576857	-1.826588	-0.160598
33	1	0	-0.233384	-2.563932	-0.191506
34	1	0	1.521582	-2.371175	-0.236505
35	1	0	0.549858	-1.327799	0.813265
36	6	0	0.508529	2.257009	-0.040098
37	1	0	0.319197	2.231318	-1.105537
38	1	0	1.690806	0.872183	-2.130734
39	6	0	-5.344025	0.132258	-0.564341
40	6	0	-4.112337	0.615205	0.199714
41	6	0	-3.290215	-1.723935	0.413657
42	6	0	-4.513551	-2.240762	-0.339838
43	6	0	-5.067624	-1.183492	-1.305006
44	1	0	-3.285558	0.820919	-0.484525
45	1	0	-4.317418	1.513474	0.788229
46	1	0	-6.202024	0.023547	0.109802
47	1	0	-5.614160	0.925348	-1.269877
48	1	0	-2.473905	-1.473211	-0.273675
49	1	0	-2.926586	-2.440765	1.154576
50	1	0	-4.195128	-3.133804	-0.888223
51	1	0	-5.293294	-2.575237	0.354751
52	1	0	-4.339905	-1.005983	-2.106600
53	1	0	-5.983004	-1.547376	-1.780833
54	6	0	-4.503767	-0.643402	2.322633

55	1	0	-4.063156	-1.378372	2.997406
56	1	0	-4.640553	0.302716	2.848439
57	1	0	-5.464220	-1.005823	1.964150
58	7	0	-3.561480	-0.423091	1.174032
59	6	0	-2.246074	0.089104	1.710963
60	1	0	-2.424814	1.036661	2.222115
61	1	0	-1.563092	0.216151	0.862250
62	1	0	-1.854558	-0.644617	2.417803

TSn_2A

SCF Done: E(RB3LYP) = -1258.69345417 A.U.

Sum of electronic and thermal Free Energies= -1258.203384 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.232054	-1.024447	-1.266254
2	6	0	-2.134723	-0.589643	-0.268238
3	6	0	-2.074991	-1.063650	1.080155
4	1	0	-1.223948	-0.492916	-2.212960
5	1	0	-2.882419	-0.707196	1.716450
6	8	0	-2.908714	0.444612	-0.620752
7	14	0	-4.510410	0.941962	-0.202650
8	6	0	-4.499831	1.815702	1.463111
9	1	0	-3.774698	2.636626	1.477973
10	1	0	-4.275481	1.144718	2.298695
11	1	0	-5.488493	2.250687	1.653283
12	6	0	-4.935755	2.133334	-1.582700
13	1	0	-5.942246	2.544521	-1.444628
14	1	0	-4.906075	1.637608	-2.558556
15	1	0	-4.233035	2.973122	-1.608721
16	6	0	-5.611575	-0.579373	-0.193071
17	1	0	-5.576510	-1.099720	-1.156293
18	1	0	-6.652321	-0.284497	-0.014397
19	1	0	-5.335276	-1.294003	0.589218
20	8	0	0.572797	-2.326320	-2.010380
21	6	0	1.209760	-3.610741	-1.912430
22	1	0	1.972248	-3.634096	-2.690750
23	1	0	0.483525	-4.410199	-2.089264
24	1	0	1.671442	-3.738712	-0.927310
25	6	0	-0.535073	-0.478417	1.867391
26	7	0	0.574184	-1.183153	1.475511
27	6	0	0.654460	-2.484892	2.119145
28	1	0	-0.159290	-3.183059	1.829977
29	1	0	0.605953	-2.421804	3.219765
30	1	0	1.595017	-2.989178	1.862494
31	1	0	-0.880165	-0.699275	2.892056
32	6	0	-0.470390	1.025867	1.630791
33	1	0	0.308103	1.466833	2.263634
34	1	0	-1.415232	1.516235	1.879754
35	1	0	-0.235074	1.253703	0.586393
36	6	0	-0.338386	-2.042889	-1.066192
37	1	0	-0.382934	-2.720131	-0.222909
38	1	0	-1.945086	-2.140519	1.186743
39	6	0	2.522607	1.978178	-0.979092
40	6	0	2.707388	0.495271	-0.669451
41	6	0	5.107717	0.906687	-0.079621
42	6	0	4.942303	2.394547	-0.383733
43	6	0	3.835910	2.640023	-1.419256
44	1	0	3.019038	-0.043876	-1.569313
45	1	0	1.811292	0.017139	-0.260426
46	1	0	2.096369	2.502049	-0.116044
47	1	0	1.770952	2.045396	-1.772824
48	1	0	5.429218	0.368601	-0.976620
49	1	0	5.840660	0.725384	0.711029
50	1	0	5.908018	2.756427	-0.752504
51	1	0	4.741102	2.954624	0.536505
52	1	0	4.146370	2.230045	-2.389699
53	1	0	3.690484	3.714461	-1.564995
54	6	0	3.377697	0.716270	1.725867
55	1	0	4.171300	0.485649	2.438584
56	1	0	2.453190	0.183132	1.972248
57	1	0	3.205999	1.789568	1.703482
58	7	0	3.812213	0.238738	0.361485
59	6	0	4.024868	-1.247071	0.452569
60	1	0	3.078278	-1.698416	0.750082
61	1	0	4.340407	-1.620644	-0.522425
62	1	0	4.798029	-1.449736	1.195521

TSn_2B

SCF Done: E(RB3LYP) = -1258.69325570 A.U.

Sum of electronic and thermal Free Energies= -1258.205532 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.649580	1.563415	-0.613224
2	6	0	-2.417170	0.588884	0.066404
3	6	0	-2.107159	0.152220	1.393441
4	1	0	-1.839022	1.714887	-1.671428
5	1	0	-2.838634	-0.530377	1.821199
6	8	0	-3.323910	-0.039900	-0.690676
7	14	0	-4.872614	-0.744161	-0.385491
8	6	0	-4.662528	-2.458426	0.359540
9	1	0	-4.031967	-3.094082	-0.271549
10	1	0	-4.230754	-2.438048	1.365539
11	1	0	-5.642073	-2.945701	0.437003
12	6	0	-5.620088	-0.838883	-2.098712
13	1	0	-6.617082	-1.292565	-2.062438
14	1	0	-5.719840	0.156747	-2.543381
15	1	0	-5.000603	-1.446649	-2.766926
16	6	0	-5.823485	0.407445	0.753837
17	1	0	-5.901048	1.412480	0.325099
18	1	0	-6.842899	0.030419	0.897928
19	1	0	-5.364156	0.494973	1.743843
20	8	0	0.113619	3.106994	-0.731168
21	6	0	0.863602	4.086370	0.005184
22	1	0	1.495831	4.596897	-0.720960
23	1	0	0.188657	4.809403	0.473776
24	1	0	1.481533	3.604809	0.771129
25	6	0	-0.526951	-0.761278	1.388060
26	7	0	0.571529	0.055963	1.308313
27	6	0	0.868558	0.706893	2.574241
28	1	0	0.095313	1.434272	2.901136
29	1	0	0.967893	-0.005969	3.411298
30	1	0	1.809490	1.268671	2.508292
31	1	0	-0.689934	-1.211076	2.382739
32	6	0	-0.641053	-1.815532	0.293692
33	1	0	0.199248	-2.515780	0.364213
34	1	0	-1.563638	-2.394731	0.386670
35	1	0	-0.629215	-1.361132	-0.702212
36	6	0	-0.651838	2.277229	-0.005811
37	1	0	-0.496443	2.293075	1.065542
38	1	0	-1.865331	0.949270	2.096289
39	6	0	4.717730	-1.309994	1.198876
40	6	0	3.494018	-1.409420	0.291558
41	6	0	4.840772	-0.539009	-1.632866
42	6	0	6.073980	-0.427369	-0.738503
43	6	0	6.029499	-1.442071	0.412301
44	1	0	3.447795	-2.396705	-0.178686

45	1	0	2.551046	-1.210489	0.814141
46	1	0	4.701202	-0.371673	1.765144
47	1	0	4.628347	-2.109937	1.941654
48	1	0	4.807291	-1.521126	-2.114454
49	1	0	4.826065	0.226188	-2.413422
50	1	0	6.949462	-0.597269	-1.374164
51	1	0	6.175269	0.592349	-0.349310
52	1	0	6.113821	-2.459215	0.006965
53	1	0	6.887100	-1.296612	1.075676
54	6	0	3.323676	0.992723	-0.349879
55	1	0	3.332609	1.675977	-1.200612
56	1	0	2.350569	1.000916	0.150505
57	1	0	4.122069	1.253772	0.340667
58	7	0	3.531147	-0.408494	-0.868056
59	6	0	2.382914	-0.711594	-1.793223
60	1	0	1.459047	-0.585510	-1.228398
61	1	0	2.478639	-1.735860	-2.155522
62	1	0	2.415155	-0.014977	-2.632653

TSn_3A

SCF Done: E(RB3LYP) = -1258.69367115 A.U.

Sum of electronic and thermal Free Energies= -1258.203719 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.552105	1.375541	-0.868392
2	6	0	2.417086	0.604117	-0.056605
3	6	0	2.204902	0.436445	1.347360
4	1	0	1.673218	1.312999	-1.945510
5	1	0	2.993285	-0.111219	1.859348
6	8	0	3.322256	-0.118498	-0.727779
7	14	0	4.921702	-0.669148	-0.371608
8	6	0	4.841307	-2.221060	0.687757
9	1	0	4.221324	-2.993109	0.219269
10	1	0	4.451444	-2.031989	1.693379
11	1	0	5.849277	-2.637512	0.803090
12	6	0	5.611319	-1.044327	-2.070869
13	1	0	6.635101	-1.428700	-1.997957
14	1	0	5.633269	-0.146023	-2.696555
15	1	0	5.006892	-1.799418	-2.584811
16	6	0	5.841429	0.723598	0.490537
17	1	0	5.848807	1.631778	-0.121860
18	1	0	6.884301	0.432054	0.662144
19	1	0	5.406887	0.974104	1.463860
20	8	0	-0.321397	2.754398	-1.180788
21	6	0	-1.108342	3.809761	-0.605556
22	1	0	-1.793680	4.140376	-1.385785
23	1	0	-0.466782	4.644567	-0.306403
24	1	0	-1.670060	3.443265	0.260701
25	6	0	0.674402	-0.531932	1.628392
26	7	0	-0.468224	0.201934	1.445702
27	6	0	-0.743666	1.088058	2.564774
28	1	0	0.017666	1.883626	2.710378
29	1	0	-0.795797	0.555758	3.530086
30	1	0	-1.701919	1.604663	2.423464
31	1	0	0.916253	-0.753647	2.681971
32	6	0	0.790729	-1.783930	0.767206
33	1	0	0.026266	-2.510715	1.064549
34	1	0	1.765126	-2.266009	0.881413
35	1	0	0.649195	-1.550555	-0.292740
36	6	0	0.541293	2.142240	-0.353658
37	1	0	0.447122	2.378689	0.698268
38	1	0	1.950547	1.347471	1.888663
39	6	0	-5.857352	-1.602853	-0.780275
40	6	0	-4.521084	-1.355128	-1.477839
41	6	0	-3.968991	0.443614	0.161309
42	6	0	-5.301113	0.220382	0.874595
43	6	0	-6.368038	-0.336775	-0.078196
44	1	0	-4.636214	-0.610292	-2.271430
45	1	0	-4.111195	-2.265861	-1.921598
46	1	0	-5.770346	-2.430050	-0.066334
47	1	0	-6.565343	-1.935894	-1.546501
48	1	0	-4.079606	1.199580	-0.622120
49	1	0	-3.170180	0.753773	0.837304
50	1	0	-5.613149	1.187559	1.283128
51	1	0	-5.170003	-0.443060	1.736801
52	1	0	-6.620778	0.422512	-0.830378
53	1	0	-7.289143	-0.554411	0.470162
54	6	0	-3.014768	-1.835450	0.468003
55	1	0	-2.210331	-1.383462	1.057761
56	1	0	-2.647661	-2.709670	-0.071814
57	1	0	-3.855220	-2.119302	1.097013
58	7	0	-3.449853	-0.805523	-0.546284
59	6	0	-2.230491	-0.419086	-1.348201
60	1	0	-1.868975	-1.305477	-1.872292
61	1	0	-2.512781	0.348616	-2.069642
62	1	0	-1.475334	-0.048325	-0.645956

TSn_3B

SCF Done: E(RB3LYP) = -1258.69362500 A.U.

Sum of electronic and thermal Free Energies= -1258.203886 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.590809	1.339874	-1.010238
2	6	0	-2.378716	0.558435	-0.132869
3	6	0	-2.228949	0.610878	1.288008
4	1	0	-1.635108	1.116373	-2.071710
5	1	0	-2.961836	0.025037	1.839069
6	8	0	-3.124992	-0.379495	-0.730330
7	14	0	-4.664704	-1.081848	-0.379598
8	6	0	-4.470622	-2.446641	0.900159
9	1	0	-3.733635	-3.191878	0.581366
10	1	0	-4.172936	-2.070162	1.884341
11	1	0	-5.427254	-2.967544	1.028019
12	6	0	-5.181564	-1.777980	-2.038546
13	1	0	-6.152903	-2.280069	-1.964171
14	1	0	-5.269182	-0.985560	-2.789107
15	1	0	-4.453779	-2.510422	-2.403967
16	6	0	-5.807793	0.284021	0.218004
17	1	0	-5.875083	1.093814	-0.516539
18	1	0	-6.819010	-0.113399	0.364956
19	1	0	-5.484208	0.715979	1.170705
20	8	0	0.067765	2.946573	-1.437161
21	6	0	0.635899	4.188505	-0.988924
22	1	0	1.329337	4.505904	-1.767431
23	1	0	-0.147184	4.943438	-0.867704
24	1	0	1.168874	4.049650	-0.041846
25	6	0	-0.599504	-0.076302	1.758774
26	7	0	0.438687	0.781909	1.515210
27	6	0	0.537038	1.841830	2.504823
28	1	0	-0.323142	2.544238	2.503689
29	1	0	0.597565	1.459315	3.538534
30	1	0	1.432768	2.450272	2.325113
31	1	0	-0.866538	-0.187522	2.823792
32	6	0	-0.489119	-1.435463	1.079207
33	1	0	0.353099	-1.991182	1.508344
34	1	0	-1.390128	-2.038452	1.221311

35	1	0	-0.321110	-1.322784	0.003007
36	6	0	-0.741332	2.318385	-0.568848
37	1	0	-0.747615	2.702654	0.443331
38	1	0	-2.137951	1.612322	1.708119
39	6	0	3.944119	-2.600170	-0.158346
40	6	0	3.082986	-1.394278	-0.529043
41	6	0	5.122876	0.021734	-0.758179
42	6	0	6.008678	-1.166180	-0.387237
43	6	0	5.349963	-2.500176	-0.765936
44	1	0	2.929889	-1.355519	-1.611758
45	1	0	2.107261	-1.404467	-0.041573
46	1	0	4.002030	-2.713527	0.930220
47	1	0	3.423862	-3.490419	-0.527505
48	1	0	4.978101	0.067157	-1.841975
49	1	0	5.549163	0.972886	-0.429716
50	1	0	6.959280	-1.037673	-0.915667
51	1	0	6.250308	-1.145426	0.681607
52	1	0	5.283762	-2.578761	-1.859303
53	1	0	5.969561	-3.335996	-0.428251
54	6	0	3.753018	0.115436	1.340672
55	1	0	4.234906	1.068921	1.562782
56	1	0	2.713363	0.126323	1.684857
57	1	0	4.315412	-0.693224	1.801186
58	7	0	3.725581	-0.058881	-0.158757
59	6	0	2.870111	1.049530	-0.722650
60	1	0	1.893121	1.009249	-0.224236
61	1	0	2.776699	0.910261	-1.800347
62	1	0	3.366346	1.999621	-0.515411

TSn_4A

SCF Done: E(RB3LYP) = -1258.69079046 A.U.

Sum of electronic and thermal Free Energies= -1258.200522 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.365073	-1.420718	0.828039
2	6	0	2.235894	-0.644971	0.029194
3	6	0	2.030956	-0.470428	-1.373109
4	1	0	1.467935	-1.355003	1.906962
5	1	0	2.805384	0.102465	-1.878476
6	8	0	3.129964	0.085825	0.712036
7	14	0	4.725198	0.642604	0.356604
8	6	0	4.639430	2.196645	-0.700305
9	1	0	4.009778	2.962475	-0.234347
10	1	0	4.257162	2.006527	-1.708657
11	1	0	5.644492	2.621902	-0.808752
12	6	0	5.415766	1.020022	2.055597
13	1	0	6.438025	1.408248	1.981620
14	1	0	5.441823	0.121445	2.680776
15	1	0	4.809197	1.772649	2.570685
16	6	0	5.655173	-0.742380	-0.507632
17	1	0	5.667400	-1.651893	0.102735
18	1	0	6.696358	-0.444077	-0.677873
19	1	0	5.222650	-0.993562	-1.481660
20	8	0	-0.524963	-2.785315	1.115439
21	6	0	-1.310175	-3.835022	0.527651
22	1	0	-1.992363	-4.179647	1.304803
23	1	0	-0.667658	-4.664096	0.214704
24	1	0	-1.875467	-3.457217	-0.331225
25	6	0	0.461985	0.465033	-1.637622
26	7	0	-0.650865	-0.308767	-1.462324
27	6	0	-0.913232	-1.180006	-2.595703
28	1	0	-0.130056	-1.949054	-2.765285
29	1	0	-0.990028	-0.628337	-3.548054
30	1	0	-1.855195	-1.723421	-2.452334
31	1	0	0.698226	0.709702	-2.686998
32	6	0	0.543882	1.701342	-0.751117
33	1	0	-0.258591	2.398963	-1.017409
34	1	0	1.495197	2.226436	-0.872507
35	1	0	0.433552	1.436659	0.305184
36	6	0	0.357608	-2.183617	0.297898
37	1	0	0.293922	-2.445334	-0.749680
38	1	0	1.791171	-1.377502	-1.927255
39	6	0	-3.559704	1.852350	-1.072152
40	6	0	-3.750815	2.111252	0.420463
41	6	0	-4.762893	-0.154183	0.693761
42	6	0	-4.576173	-0.428011	-0.796072
43	6	0	-4.609374	0.871950	-1.610473
44	1	0	-4.719500	2.583166	0.613949
45	1	0	-2.966240	2.751365	0.831688
46	1	0	-2.554530	1.460993	-1.268551
47	1	0	-3.634881	2.822561	-1.575464
48	1	0	-5.742969	0.295671	0.880333
49	1	0	-4.680562	-1.061633	1.297167
50	1	0	-5.382339	-1.104400	-1.100510
51	1	0	-3.633486	-0.956704	-0.970707
52	1	0	-5.611427	1.319248	-1.556308
53	1	0	-4.414724	0.658173	-2.665146
54	6	0	-2.355855	0.218989	1.277167
55	1	0	-2.400400	-0.711229	1.845804
56	1	0	-1.692087	0.923234	1.781116
57	1	0	-1.974357	0.027070	0.266067
58	7	0	-3.740093	0.830251	1.256083
59	6	0	-4.131743	1.170404	2.667171
60	1	0	-3.418891	1.892302	3.067548
61	1	0	-5.134984	1.598172	2.671882
62	1	0	-4.112440	0.260843	3.269059

TSn_4B

SCF Done: E(RB3LYP) = -1258.69079066 A.U.

Sum of electronic and thermal Free Energies= -1258.200514 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.365299	1.421066	0.827798
2	6	0	2.235996	0.645004	0.029125
3	6	0	2.030952	0.470051	-1.373118
4	1	0	1.468260	1.355704	1.906732
5	1	0	2.805341	-0.103014	-1.878348
6	8	0	3.130055	-0.085668	0.712111
7	14	0	4.725214	-0.642657	0.356657
8	6	0	4.639158	-2.196789	-0.700105
9	1	0	4.009416	-2.962477	-0.234035
10	1	0	4.256833	-2.006678	-1.708437
11	1	0	5.644139	-2.622225	-0.808600
12	6	0	5.415844	-1.019955	2.055648
13	1	0	6.438138	-1.408087	1.981659
14	1	0	5.441833	-0.121346	2.680784
15	1	0	4.809361	-1.772617	2.570785
16	6	0	5.655296	0.742130	-0.507780
17	1	0	5.667978	1.651593	0.102654
18	1	0	6.696341	0.443544	-0.678381
19	1	0	5.222532	0.993515	-1.481649
20	8	0	-0.524619	2.785891	1.114904
21	6	0	-1.309873	3.835401	0.526825
22	1	0	-1.992055	4.180240	1.303886
23	1	0	-0.667386	4.664397	0.213612
24	1	0	-1.875172	3.457316	-0.331924

25	6	0	0.461989	-0.465444	-1.637304
26	7	0	-0.650854	0.308437	-1.462293
27	6	0	-0.913163	1.179361	-2.595921
28	1	0	-0.130086	1.948505	-2.765536
29	1	0	-0.989689	0.627465	-3.548164
30	1	0	-1.855242	1.722652	-2.452839
31	1	0	0.698217	-0.710508	-2.686593
32	6	0	0.543810	-1.701446	-0.750361
33	1	0	-0.258652	-2.399151	-1.016465
34	1	0	1.495125	-2.226597	-0.871496
35	1	0	0.433402	-1.436384	0.305838
36	6	0	0.357836	2.183855	0.297495
37	1	0	0.294041	2.445171	-0.750177
38	1	0	1.791214	1.376991	-1.927509
39	6	0	-3.559455	-1.852616	-1.071705
40	6	0	-3.750457	-2.111088	0.420999
41	6	0	-4.763388	0.154063	0.693525
42	6	0	-4.576695	0.427486	-0.796382
43	6	0	-4.609462	-0.872755	-1.610354
44	1	0	-4.718950	-2.583325	0.614655
45	1	0	-2.965621	-2.750748	0.832430
46	1	0	-2.554408	-1.460999	-1.268242
47	1	0	-3.634315	-2.823024	-1.574685
48	1	0	-5.743307	-0.296100	0.880178
49	1	0	-4.681435	1.061732	1.296654
50	1	0	-5.383055	1.103531	-1.101070
51	1	0	-3.634164	0.956412	-0.971155
52	1	0	-5.611366	-1.320366	-1.556026
53	1	0	-4.414892	-0.659270	-2.665101
54	6	0	-2.356239	-0.218023	1.277178
55	1	0	-2.401228	0.712461	1.845346
56	1	0	-1.692275	-0.921758	1.781578
57	1	0	-1.974649	-0.026492	0.266038
58	7	0	-3.740250	-0.829813	1.256208
59	6	0	-4.131847	-1.169661	2.667385
60	1	0	-3.418743	-1.891160	3.068033
61	1	0	-5.134927	-1.597806	2.672182
62	1	0	-4.112920	-0.259897	3.268979

Realistic models

TSend

SCF Done: E(RB3LYP) = -1311.20134819 A.U.

Sum of electronic and thermal Free Energies= -1310.830813 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.155131	-1.415245	1.456412
2	6	0	-0.851895	-1.064503	0.284923
3	6	0	-0.200338	-0.593317	-0.907381
4	1	0	-0.733257	-1.577682	2.361618
5	1	0	-0.882218	-0.457732	-1.746749
6	8	0	-2.188389	-1.012570	0.413428
7	14	0	-3.507593	-1.437865	-0.589232
8	6	0	-3.823675	-0.142257	-1.917456
9	1	0	-3.854706	0.864586	-1.486340
10	1	0	-3.062812	-0.147427	-2.706787
11	1	0	-4.793397	-0.334574	-2.396196
12	6	0	-4.940531	-1.508125	0.620990
13	1	0	-5.875810	-1.771928	0.110847
14	1	0	-4.761001	-2.254052	1.404234
15	1	0	-5.087116	-0.537770	1.110414
16	6	0	-3.137412	-3.120711	-1.352024
17	1	0	-2.966478	-3.879536	-0.578830
18	1	0	-3.981003	-3.456903	-1.968975
19	1	0	-2.249967	-3.092495	-1.995917
20	8	0	1.795687	-1.678191	2.713149
21	6	0	3.199152	-1.995251	2.712283
22	1	0	3.551077	-1.807680	3.727458
23	1	0	3.336022	-3.053434	2.461222
24	1	0	3.737399	-1.362881	2.002284
25	6	0	0.577195	1.005078	-0.645726
26	7	0	1.748019	0.917116	0.072964
27	1	0	0.698582	1.246831	-1.713518
28	6	0	1.215059	-1.480693	1.528234
29	1	0	1.867568	-1.447971	0.663530
30	1	0	0.668384	-1.181364	-1.208689
31	6	0	-0.454434	1.925668	-0.034992
32	6	0	-1.391411	2.572354	-0.852763
33	6	0	-0.487761	2.167842	1.345574
34	6	0	-2.350003	3.431899	-0.308544
35	1	0	-1.361837	2.415054	-1.930176
36	6	0	-1.448945	3.020145	1.893706
37	1	0	0.266046	1.702608	1.971923
38	6	0	-2.385900	3.653939	1.070961
39	1	0	-3.058725	3.936050	-0.961883
40	1	0	-1.459493	3.199889	2.966423
41	1	0	-3.126710	4.325349	1.498595
42	6	0	2.896694	0.525133	-0.580467
43	6	0	4.117947	0.646777	0.142753
44	6	0	2.994640	0.004501	-1.901766
45	6	0	5.338204	0.278200	-0.407185
46	1	0	4.061289	1.069629	1.143313
47	6	0	4.228769	-0.367816	-2.445171
48	1	0	2.111013	-0.087480	-2.526067
49	6	0	5.408717	-0.241811	-1.710525
50	1	0	6.248786	0.404049	0.175626
51	1	0	4.262732	-0.757891	-3.460803
52	1	0	6.363772	-0.529710	-2.141693

TSexo

SCF Done: E(RB3LYP) = -1311.20110174 A.U.

Sum of electronic and thermal Free Energies= -1310.832145 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.577327	1.162951	1.701790
2	6	0	1.166386	0.082354	1.021944
3	6	0	0.405926	-1.069948	0.661125
4	1	0	1.137454	2.088792	1.790405
5	1	0	0.959669	-1.883543	0.198486
6	8	0	2.421697	0.287146	0.567100
7	14	0	3.703909	-0.746868	0.121220
8	6	0	3.378196	-1.507645	-1.573289
9	1	0	3.156695	-0.733828	-2.318626
10	1	0	2.542640	-2.217127	-1.568276
11	1	0	4.267281	-2.052010	-1.918828
12	6	0	5.174938	0.417074	0.048202
13	1	0	6.087515	-0.117567	-0.245057
14	1	0	5.357389	0.886690	1.022069
15	1	0	5.006176	1.218103	-0.681476
16	6	0	3.927923	-2.070950	1.442383
17	1	0	4.095182	-1.618393	2.427485
18	1	0	4.801233	-2.695088	1.211231
19	1	0	3.060043	-2.735646	1.522554
20	8	0	-1.320048	2.261515	2.533659
21	6	0	-2.687899	2.141327	2.946514

22	1	0	-3.021865	3.151750	3.184676
23	1	0	-2.762094	1.506317	3.837850
24	1	0	-3.290906	1.726638	2.132659
25	6	0	-0.939299	-0.642359	-0.604254
26	7	0	-1.621429	0.504447	-0.320843
27	1	0	-0.304963	-0.631927	-1.499953
28	6	0	-0.745657	1.143755	2.079454
29	1	0	-1.346582	0.243844	2.120956
30	1	0	-0.248978	-1.442665	1.444785
31	6	0	-1.215796	1.690961	-0.919808
32	6	0	-2.121289	2.780182	-0.861580
33	6	0	0.016427	1.913988	-1.583683
34	6	0	-1.819868	4.011628	-1.433133
35	1	0	-3.077576	2.616839	-0.371281
36	6	0	0.314240	3.154265	-2.151824
37	1	0	0.756012	1.122579	-1.648583
38	6	0	-0.595148	4.213238	-2.084606
39	1	0	-2.544447	4.821329	-1.375976
40	1	0	1.271731	3.294015	-2.650124
41	1	0	-0.357545	5.175272	-2.531134
42	6	0	-1.756336	-1.911598	-0.546633
43	6	0	-1.320380	-3.055812	-1.231063
44	6	0	-2.953783	-1.982931	0.179759
45	6	0	-2.053227	-4.244820	-1.186251
46	1	0	-0.404006	-3.012140	-1.818064
47	6	0	-3.684490	-3.171843	0.233466
48	1	0	-3.317128	-1.085510	0.670698
49	6	0	-3.237135	-4.309566	-0.446534
50	1	0	-1.702241	-5.116813	-1.733135
51	1	0	-4.613999	-3.207461	0.797320
52	1	0	-3.810956	-5.232217	-0.409784

CPs_1A_real

SCF Done: E(RB3LYP) = -1191.29265932 A.U.

Sum of electronic and thermal Free Energies= -1190.958947 A.U.

[SMD(CH_2Cl_2)-B3LYP/6-311+G**]

SCF Done: E(RB3LYP) = -1191.55036152 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.082856	-1.133314	-0.437460
2	7	0	-1.122681	-1.166385	0.416632
3	1	0	-2.049329	-1.744524	-1.350489
4	6	0	3.873407	0.499226	-0.297197
5	6	0	2.725972	0.372884	0.709923
6	6	0	2.065997	2.982681	-0.042370
7	6	0	3.273106	2.895796	-0.985437
8	6	0	4.368356	1.943244	-0.477581
9	1	0	2.379485	-0.655088	0.824753
10	1	0	2.988573	0.788794	1.688348
11	1	0	4.684922	-0.136172	0.073922
12	1	0	3.563336	0.071190	-1.258142
13	1	0	1.289434	3.654019	-0.418292
14	1	0	2.355592	3.293431	0.966983
15	1	0	2.938638	2.592745	-1.985423
16	1	0	3.672989	3.910649	-1.085496
17	1	0	5.203714	1.951777	-1.183980
18	1	0	4.761994	2.316674	0.477292
19	16	0	1.272204	1.325058	0.097709
20	6	0	0.215887	1.500314	1.567699
21	1	0	-0.523720	2.270686	1.338217
22	1	0	-0.292099	0.539317	1.691783
23	1	0	0.818801	1.780017	2.433677
24	6	0	0.036159	-1.923706	0.156042
25	6	0	0.675673	-1.935258	-1.099132
26	6	0	0.626063	-2.615580	1.229793
27	6	0	1.867608	-2.642810	-1.274981
28	1	0	0.249006	-1.374383	-1.925616
29	6	0	1.808425	-3.333077	1.042269
30	1	0	0.131249	-2.598738	2.196134
31	6	0	2.438286	-3.345313	-0.208740
32	1	0	2.349124	-2.646918	-2.248671
33	1	0	2.239608	-3.883355	1.873100
34	1	0	3.360056	-3.900394	-0.351065
35	6	0	-3.278587	-0.306372	-0.266760
36	6	0	-4.205672	-0.228063	-1.320836
37	6	0	-3.527800	0.407925	0.921893
38	6	0	-5.349770	0.562130	-1.200582
39	1	0	-4.028354	-0.787776	-2.235831
40	6	0	-4.672271	1.189908	1.041913
41	1	0	-2.831776	0.315305	1.748999
42	6	0	-5.583574	1.272916	-0.020695
43	1	0	-6.058980	0.617222	-2.020347
44	1	0	-4.867982	1.726669	1.965325
45	1	0	-6.477230	1.881439	0.078476

TSs_1A_real

SCF Done: E(RB3LYP) = -1945.80648978 A.U.

Sum of electronic and thermal Free Energies= -1945.264839 A.U.

[SMD(CH_2Cl_2)-B3LYP/6-311+G**]

SCF Done: E(RB3LYP) = -1946.18350797 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.533466	2.143682	-0.736879
2	6	0	-2.706632	1.085321	0.198654
3	6	0	-1.791828	0.791246	1.238264
4	1	0	-3.226167	2.189891	-1.570771
5	1	0	-2.101033	0.035738	1.953892
6	8	0	-3.721027	0.271712	-0.092980
7	14	0	-4.757236	-0.746799	0.837331
8	6	0	-3.856354	-2.331446	1.274362
9	1	0	-3.390886	-2.772150	0.387789
10	1	0	-3.073785	-2.178420	2.023784
11	1	0	-4.567872	-3.059705	1.681507
12	6	0	-6.172057	-1.065982	-0.341161
13	1	0	-6.928100	-1.708567	0.124035
14	1	0	-6.657420	-0.129868	-0.635890
15	1	0	-5.816861	-1.565569	-1.248797
16	6	0	-5.272053	0.225005	2.357426
17	1	0	-5.761947	1.163049	2.075077
18	1	0	-5.982415	-0.356288	2.956623
19	1	0	-4.417755	0.467149	2.998176
20	8	0	-1.362934	3.960690	-1.625782
21	6	0	-0.480665	5.070745	-1.351674
22	1	0	-0.252761	5.519221	-2.318123
23	1	0	-0.996210	5.798773	-0.717473
24	1	0	0.439169	4.725387	-0.872200
25	6	0	-0.185395	-0.012511	0.404040
26	7	0	0.467358	0.866024	-0.389939
27	1	0	0.239462	-0.245121	1.389798
28	6	0	-1.524592	3.057746	-0.663452
29	1	0	-0.835932	3.115738	0.175323
30	1	0	-1.281680	1.635201	1.693660
31	6	0	5.053752	-0.628556	1.030368
32	6	0	4.236748	-0.275403	-0.216957
33	6	0	3.636073	-2.999520	-0.335345
34	6	0	4.506209	-3.133751	0.921212

35	6	0	5.606711	-2.062961	1.009124
36	1	0	3.837836	0.740428	-0.185715
37	1	0	4.810109	-0.418939	-1.139020
38	1	0	5.877036	0.092060	1.082773
39	1	0	4.442590	-0.462780	1.926079
40	1	0	2.845600	-3.753391	-0.382118
41	1	0	4.232954	-3.043794	-1.252379
42	1	0	3.869752	-3.097868	1.814531
43	1	0	4.954493	-4.132992	0.898577
44	1	0	6.199832	-2.234172	1.912568
45	1	0	6.292143	-2.176153	0.158332
46	16	0	2.766174	-1.379288	-0.311111
47	6	0	2.196260	-1.205422	-2.026450
48	1	0	1.509379	-2.032867	-2.216260
49	1	0	1.637521	-0.265100	-2.049068
50	1	0	3.048900	-1.224073	-2.707922
51	6	0	1.364688	1.765099	0.162787
52	6	0	1.638435	1.949222	1.543098
53	6	0	2.108553	2.556740	-0.752785
54	6	0	2.619914	2.851092	1.967179
55	1	0	1.090266	1.387703	2.292817
56	6	0	3.083143	3.451225	-0.321176
57	1	0	1.886072	2.443764	-1.810703
58	6	0	3.355738	3.603209	1.047252
59	1	0	2.804898	2.969661	3.031644
60	1	0	3.634241	4.037177	-1.052111
61	1	0	4.112558	4.303233	1.385824
62	6	0	-0.660128	-1.252396	-0.285423
63	6	0	-0.462077	-2.502569	0.318942
64	6	0	-1.220864	-1.202972	-1.571048
65	6	0	-0.795672	-3.684140	-0.351392
66	1	0	-0.042177	-2.551408	1.321453
67	6	0	-1.570075	-2.378867	-2.235491
68	1	0	-1.362794	-0.236765	-2.043122
69	6	0	-1.350554	-3.624877	-1.633104
70	1	0	-0.638207	-4.644457	0.131317
71	1	0	-2.011461	-2.326685	-3.226526
72	1	0	-1.619524	-4.538373	-2.154769

CPn_2B_real

SCF Done: E(RB3LYP) = -887.794972841 A.U.

Sum of electronic and thermal Free Energies= -887.411200 A.U.

[SMD(CH_2Cl_2)-B3LYP/6-311+G**]

SCF Done: E(RB3LYP) = -1191.55036152 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.829668	-1.492700	-0.120633
2	7	0	-0.735691	-1.201674	0.487596
3	1	0	-1.919600	-2.403601	-0.728333
4	6	0	2.804913	0.515901	-0.893719
5	6	0	1.397863	1.085398	-1.034160
6	6	0	2.111191	3.214878	0.046069
7	6	0	3.536298	2.681909	0.187646
8	6	0	3.857972	1.632265	-0.886327
9	1	0	1.294409	1.624399	-1.981009
10	1	0	0.629948	0.315115	-0.978436
11	1	0	2.875129	-0.108523	0.003020
12	1	0	2.959226	-0.163615	-1.737376
13	1	0	1.990077	3.733676	-0.909707
14	1	0	1.845596	3.906008	0.850054
15	1	0	4.209546	3.541546	0.105877
16	1	0	3.691971	2.268303	1.189948
17	1	0	3.883185	2.116992	-1.871531
18	1	0	4.853846	1.214129	-0.715063
19	6	0	0.982055	1.446193	1.409468
20	1	0	0.718368	2.207740	2.144957
21	1	0	0.222839	0.662455	1.360160
22	1	0	1.942685	1.006739	1.662511
23	7	0	1.060973	2.107789	0.054242
24	6	0	-0.289604	2.699098	-0.250294
25	1	0	-1.034037	1.901757	-0.238086
26	1	0	-0.260168	3.171727	-1.232779
27	1	0	-0.529610	3.442754	0.511175
28	6	0	0.413375	-2.007106	0.331592
29	6	0	0.808416	-2.546314	-0.906508
30	6	0	1.243327	-2.186009	1.451716
31	6	0	1.999247	-3.268617	-1.010094
32	1	0	0.196170	-2.381276	-1.788850
33	6	0	2.424739	-2.920140	1.344334
34	1	0	0.932461	-1.769555	2.405403
35	6	0	2.810396	-3.460669	0.112286
36	1	0	2.294455	-3.679259	-1.971185
37	1	0	3.044236	-3.072980	2.222989
38	1	0	3.733304	-4.025549	0.028327
39	6	0	-3.024115	-0.645844	-0.052551
40	6	0	-4.090020	-0.898470	-0.933204
41	6	0	-3.134263	0.412441	0.871271
42	6	0	-5.231233	-0.094701	-0.913401
43	1	0	-4.021975	-1.724398	-1.636681
44	6	0	-4.276708	1.207031	0.895484
45	1	0	-2.332576	0.573764	1.584865
46	6	0	-5.325396	0.959965	-0.001937
47	1	0	-6.047104	-0.296043	-1.600304
48	1	0	-4.365080	2.008903	1.622582
49	1	0	-6.216985	1.578945	0.022378

TSn_2B_real

SCF Done: E(RB3LYP) = -1642.30799980 A.U.

Sum of electronic and thermal Free Energies= -1641.717050 A.U.

[SMD(CH_2Cl_2)-B3LYP/6-311+G**]

SCF Done: E(RB3LYP) = -1642.68006911 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.256071	1.913668	1.242491
2	6	0	2.655025	1.110045	0.140788
3	6	0	1.929958	1.020831	-1.075026
4	1	0	2.799194	1.790523	2.173709
5	1	0	2.408749	0.461378	-1.873556
6	8	0	3.672478	0.290539	0.406498
7	14	0	4.969690	-0.347738	-0.535167
8	6	0	4.375885	-1.812723	-1.543333
9	1	0	3.859436	-2.540417	-0.910698
10	1	0	3.695173	-1.524733	-2.350681
11	1	0	5.238029	-2.312632	-2.001066
12	6	0	6.192973	-0.877455	0.774997
13	1	0	7.087874	-1.316387	0.319629
14	1	0	6.506491	-0.026701	1.388686
15	1	0	5.747953	-1.628384	1.436708
16	6	0	5.599015	1.046735	-1.620725
17	1	0	5.903832	1.908479	-1.017343
18	1	0	6.470835	0.716026	-2.196889
19	1	0	4.838626	1.382765	-2.333565
20	8	0	0.823793	3.434490	2.290987
21	6	0	-0.046981	4.573836	2.117474
22	1	0	-0.499384	4.758808	3.091358
23	1	0	0.547036	5.441560	1.814088

24	1	0	-0.822499	4.360793	1.376904
25	6	0	0.302923	0.007532	-0.706479
26	7	0	-0.553966	0.693747	0.087931
27	1	0	0.073918	-0.072618	-1.778658
28	6	0	1.208717	2.786993	1.195349
29	1	0	0.671865	3.020689	0.280136
30	1	0	1.443660	1.928938	-1.421552
31	6	0	-4.156715	-0.465129	-1.237123
32	6	0	-3.111568	-1.516769	-0.878177
33	6	0	-4.683619	-2.548483	0.763012
34	6	0	-5.750004	-1.512707	0.410270
35	6	0	-5.579618	-0.996148	-1.025148
36	1	0	-3.210007	-2.394935	-1.523946
37	1	0	-2.096565	-1.127912	-0.951651
38	1	0	-3.987290	0.450488	-0.662856
39	1	0	-3.988576	-0.192721	-2.283828
40	1	0	-4.784962	-3.429752	0.122146
41	1	0	-4.748899	-2.870865	1.805437
42	1	0	-6.723395	-1.997438	0.540202
43	1	0	-5.725263	-0.680220	1.121998
44	1	0	-5.780490	-1.812504	-1.732272
45	1	0	-6.312361	-0.210752	-1.231261
46	6	0	-2.909982	-0.964994	1.549557
47	1	0	-2.932779	-1.405111	2.547521
48	1	0	-1.917374	-0.570433	1.303782
49	1	0	-3.635197	-0.159164	1.481628
50	7	0	-3.261064	-2.042708	0.551325
51	6	0	-2.302066	-3.187510	0.745798
52	1	0	-1.285023	-2.823386	0.611216
53	1	0	-2.521989	-3.965131	0.013603
54	1	0	-2.426684	-3.581508	1.755334
55	6	0	-1.379642	1.662045	-0.461621
56	6	0	-1.406245	2.080212	-1.816715
57	6	0	-2.300843	2.286586	0.420682
58	6	0	-2.326074	3.036959	-2.257466
59	1	0	-0.714468	1.656894	-2.537936
60	6	0	-3.212935	3.236833	-0.026165
61	1	0	-2.259937	2.009278	1.470640
62	6	0	-3.241278	3.617770	-1.376336
63	1	0	-2.320605	3.333668	-3.302985
64	1	0	-3.903215	3.691888	0.679702
65	1	0	-3.950155	4.360934	-1.726552
66	6	0	0.764704	-1.304112	-0.152479
67	6	0	0.926875	-2.408297	-1.000610
68	6	0	0.996351	-1.466316	1.223670
69	6	0	1.295403	-3.656438	-0.488634
70	1	0	0.759682	-2.293038	-2.069354
71	6	0	1.378676	-2.707086	1.734878
72	1	0	0.867982	-0.610508	1.877799
73	6	0	1.523247	-3.809359	0.882068
74	1	0	1.412371	-4.502759	-1.159200
75	1	0	1.566227	-2.816534	2.799192
76	1	0	1.818047	-4.774851	1.282127
