Supporting information

Title: Modeling S_N2 Reactions in Methanol Solution by Ab Initio Calculation of Nucleophile-Solvent-Substrate Clusters

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Description: Simple schematic diagrams depicting the optimized geometry for the for the stationary structures reported in the manuscript (Figs. S1-S3). The Cartesian coordinates, total energies (a.u.), vibrational zero-point energies (a.u.) enthalpies (a.u.) and free energies (a.u.) for the stationary structures reported in the manuscript are included in this supporting information. The order of the stationary points is based on the protocols given in the paper. All of the results shown here are from MP2 calculations, and the 6-31G* basis set was used for the C, H atoms, the 6-31+G* for the O atoms and lanl2dz with a *d* polarization of 0.266 for the I atoms.

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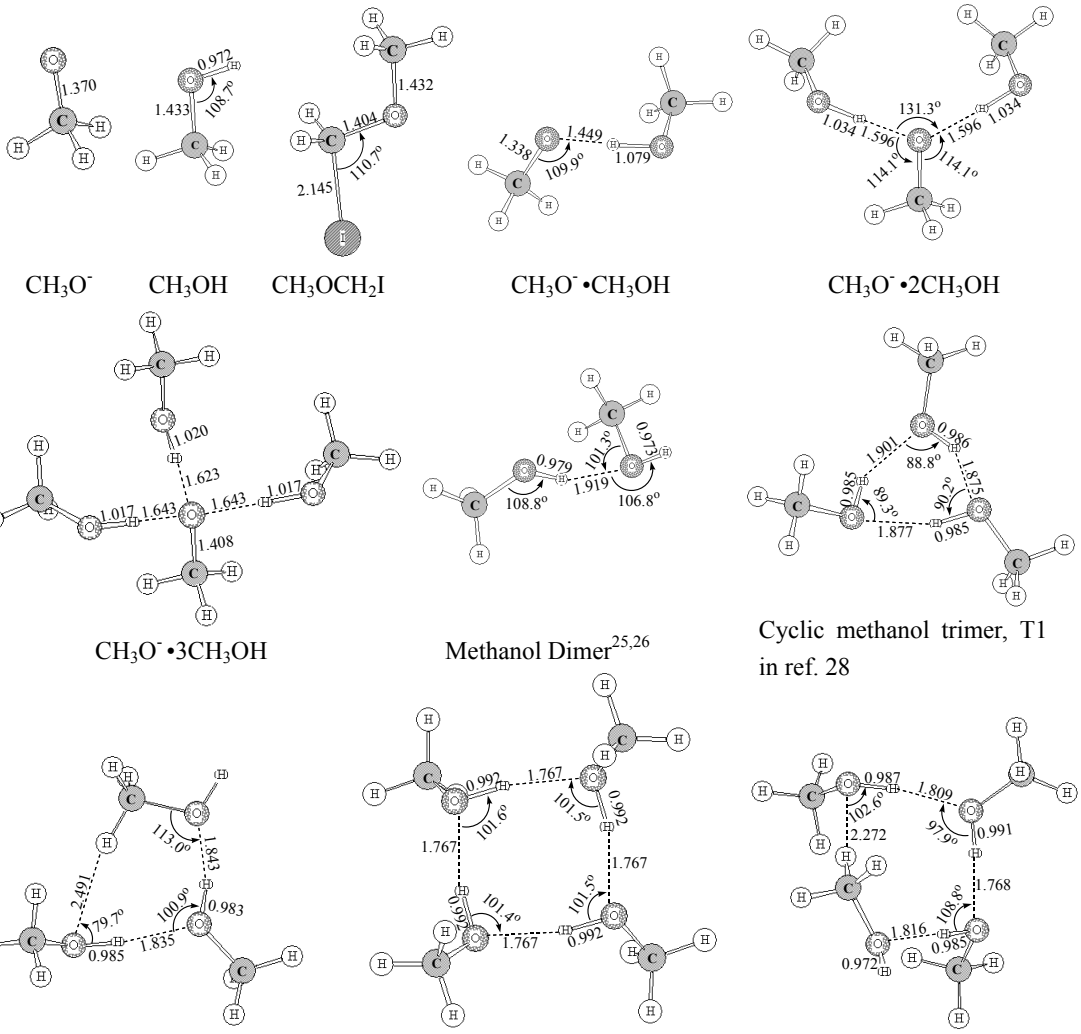

CH_3O^- CH_3OH CH_3OCH_2I $CH_3O^- \bullet CH_3OH$ $CH_3O^- \bullet 2CH_3OH$

$CH_3O^- \bullet 3CH_3OH$ Methanol Dimer[25,26] Cyclic methanol trimer, T1 in ref. 28

Open methanol trimer, T3 in ref 28. Cyclic methanol tetramer, S4 in ref 29. Open methanol tetramer

Figure 1S. Simple schematic diagrams showing the optimized structures for all the separated reactants and methanol solvated methoxide ion complexes, $CH_3O^- \bullet (CH_3OH)_n$ (n=1,2,3) and methanol clusters $(CH_3OH)_n$ (n=1,2,3,4) obtained at the MP2/BS1 level of theory.

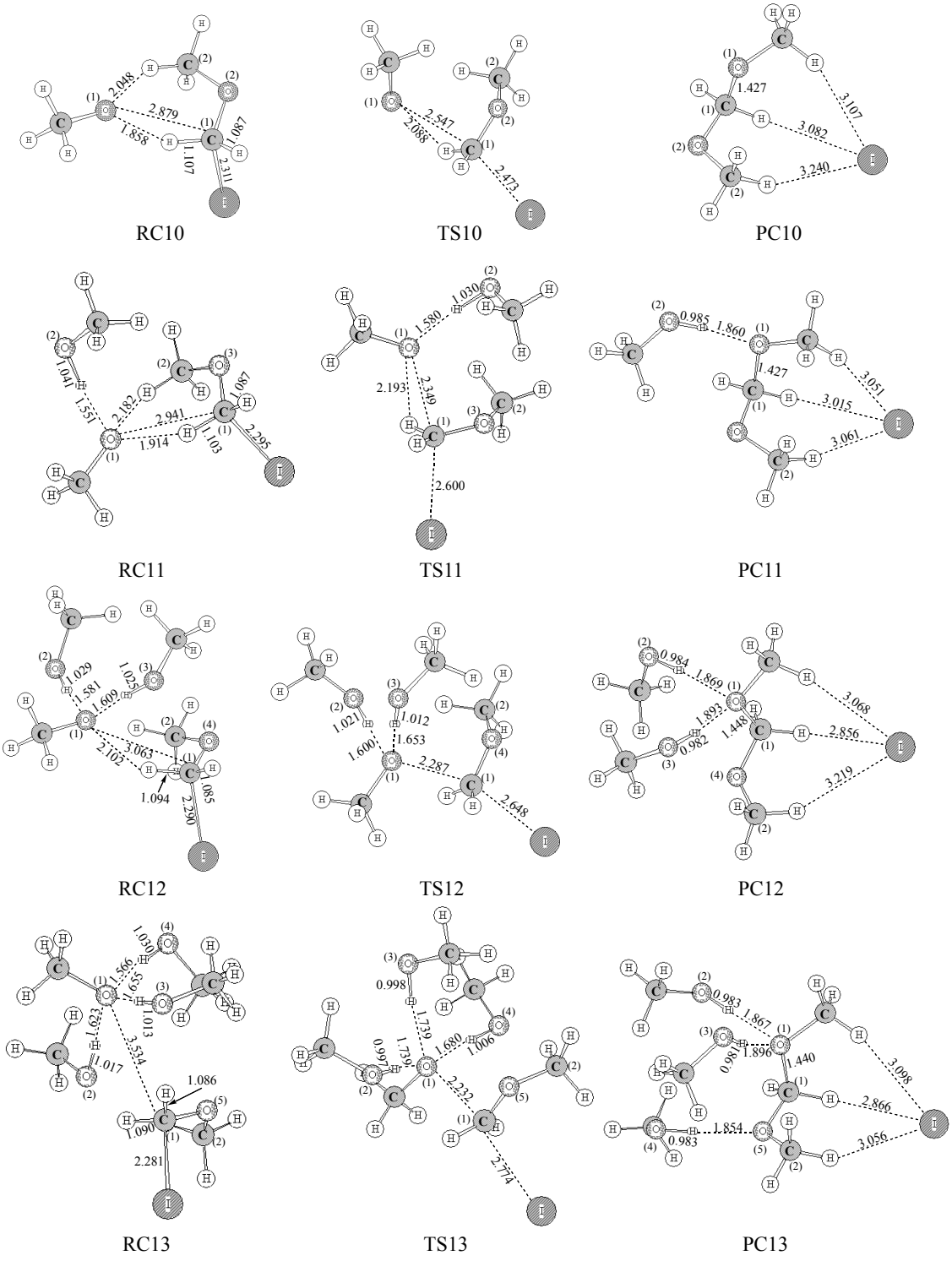

Figure 2S. Simple schematic diagrams of the optimized structures obtained from the MP2/BS1 ab initio calculations for the reactant complexes, transition states and product complexes of the reactions of $CH_3OCH_2I + CH_3O^- + (CH_3OH)_n \rightarrow CH_3OCH_2OCH_3 + I^- + (CH_3OH)_n$ where n=0,1,2,3.

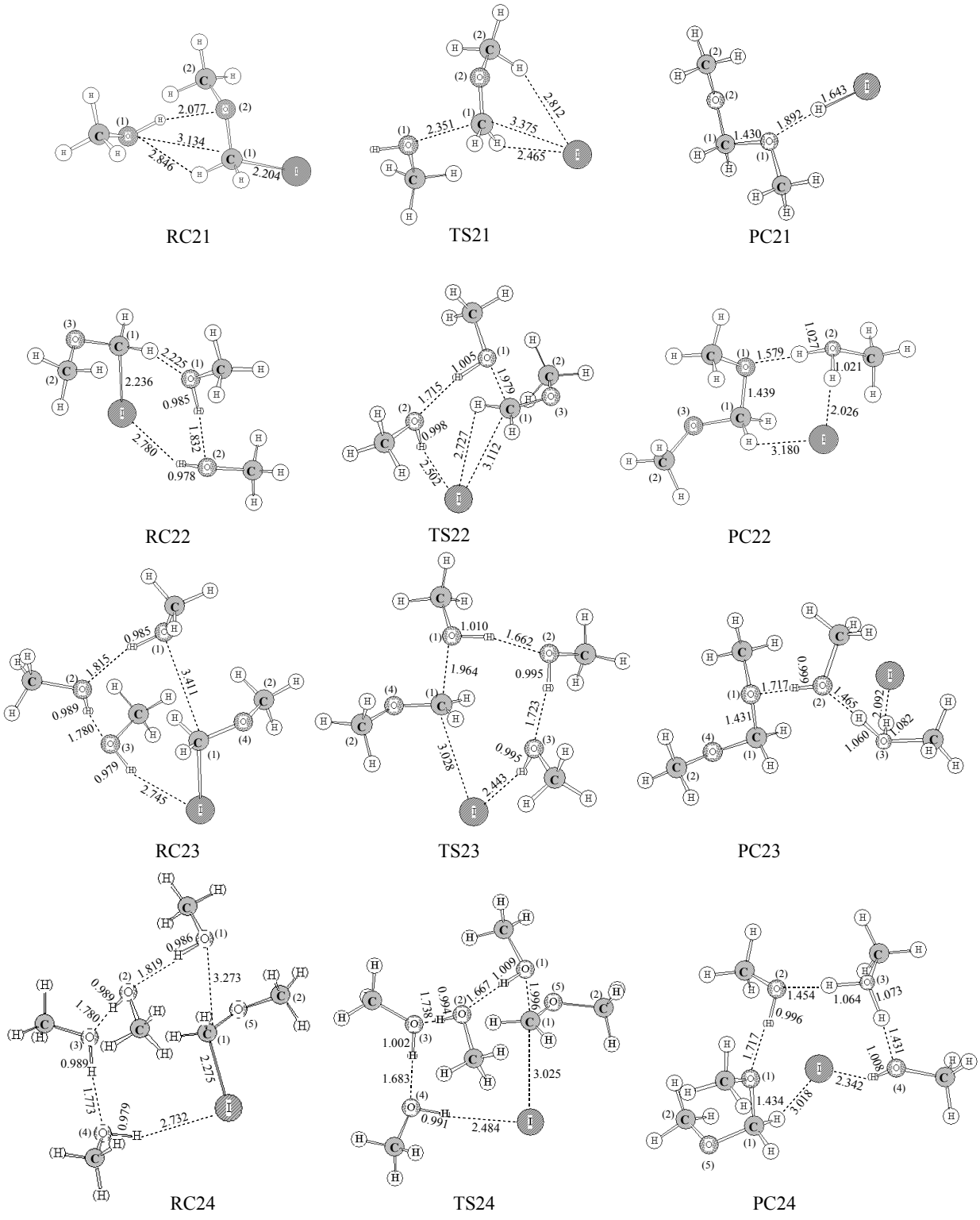

Figure 3S. Simple schematic diagrams of the optimized structures obtained from the MP2/BS1 ab initio calculations for the reactant complexes, transition states and product complexes of the reactions of $CH_3OCH_2I + (CH_3OH)_n \rightarrow CH_3OCH_2OCH_3 + HI + (CH_3OH)_n$ where n=1,2,3,4.

RC10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.399937	0.509544	0.902427
2	8	0	-0.546235	1.824501	0.578386
3	1	0	-1.222681	-0.140659	0.546528
4	1	0	-0.128628	0.430846	1.952421
5	53	0	1.494482	-0.376443	-0.080827
6	6	0	-1.206573	2.014469	-0.697251
7	1	0	-2.078286	1.352006	-0.757212
8	1	0	-1.482225	3.069893	-0.721739
9	1	0	-0.489331	1.799038	-1.497870
10	8	0	-2.948483	-0.381168	-0.099113
11	6	0	-3.918540	-1.366301	-0.040258
12	1	0	-3.807670	-2.055909	0.829414
13	1	0	-4.955499	-0.965422	0.043040
14	1	0	-3.935168	-2.031280	-0.934469

E(MP2) = -279.9650537
Zero-point correction = 0.111835
Sum of electronic and zero-point Energies = -279.853219
Sum of electronic and thermal Free Energies = -279.892452
No imaginary frequency

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.730038	-0.321355	0.240362
2	8	0	-1.172660	0.853786	0.691413
3	1	0	-0.983947	-0.608879	-0.768383
4	1	0	-0.740131	-1.090789	0.998940
5	53	0	1.721941	-0.136337	-0.020856
6	6	0	-1.539159	1.748442	-0.375577
7	1	0	-2.267830	1.225950	-1.001733
8	1	0	-1.970655	2.624914	0.106825
9	1	0	-0.637452	2.026703	-0.932578
10	8	0	-3.039446	-0.948989	-0.630876
11	6	0	-4.041962	-0.570274	0.241906
12	1	0	-3.762601	0.289053	0.903374
13	1	0	-4.978645	-0.242985	-0.268179
14	1	0	-4.357829	-1.377364	0.942650

E(MP2) = -279.9587691
Zero-point correction = 0.111453
Sum of electronic and zero-point Energies = -279.847316
Sum of electronic and thermal Free Energies = -279.884115
One imaginary frequency of -173.4891

PC10

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.061137	-1.786660	-0.658403
2	8	0	2.764029	-1.212155	0.458059
3	6	0	2.278352	0.065266	0.768174
4	8	0	2.644795	0.974393	-0.269269
5	6	0	1.756489	2.098824	-0.316050
6	53	0	-1.775778	-0.039992	0.018091
7	1	0	1.184426	0.055723	0.870859
8	1	0	2.766880	0.351150	1.707841
9	1	0	2.391294	-1.327767	-1.594242
10	1	0	2.312670	-2.848581	-0.656120
11	1	0	0.981170	-1.646741	-0.543206
12	1	0	0.715849	1.768696	-0.401173
13	1	0	1.869540	2.727367	0.578588
14	1	0	2.047946	2.677224	-1.194019

E(MP2) = -280.051359
Zero-point correction = 0.117167
Sum of electronic and zero-point Energies = -279.934192
Sum of electronic and thermal Free Energies = -279.971379
No imaginary frequency

RC11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.117274	-0.514292	-0.632231
2	8	0	-0.248084	-1.640833	0.043426
3	6	0	-0.698007	-1.371665	1.391773
4	8	0	-2.085273	1.219786	0.258136
5	6	0	-2.443043	2.566956	0.183493
6	53	0	2.246635	0.143731	-0.082992
7	1	0	-0.503012	0.367457	-0.400646
8	1	0	0.239855	-0.756897	-1.684958
9	1	0	-1.329790	-0.479125	1.400608
10	1	0	-1.254880	-2.257939	1.694994
11	1	0	0.179873	-1.237927	2.034397
12	1	0	-3.323280	2.746730	-0.467551
13	1	0	-2.701714	3.001204	1.170427
14	1	0	-1.626976	3.195321	-0.224608
15	8	0	-4.132944	-0.362743	0.256420
16	1	0	-3.343176	0.313251	0.306363
17	6	0	-3.960452	-1.078536	-0.951206
18	1	0	-4.722799	-1.864854	-0.996773
19	1	0	-4.079214	-0.435871	-1.836984
20	1	0	-2.970782	-1.553593	-1.011540

E(MP2) = -395.356139
Zero-point correction = 0.166046
Sum of electronic and zero-point Energies = -395.190093
Sum of electronic and thermal Free Energies = -395.236958
No imaginary frequency

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160165	0.289324	-0.100529
2	8	0	-0.636430	-0.938464	-0.097406
3	6	0	-0.868291	-1.461733	1.225514
4	8	0	-2.277295	1.162448	0.419959
5	6	0	-2.636300	2.474062	0.104791
6	53	0	2.425631	0.020287	-0.110220
7	1	0	-0.139525	0.864344	0.808860
8	1	0	-0.186673	0.779047	-1.059870
9	1	0	-1.517622	-0.769151	1.762448
10	1	0	-1.366860	-2.417903	1.079909
11	1	0	0.098150	-1.597544	1.722230
12	1	0	-3.143173	2.561383	-0.877796
13	1	0	-3.324390	2.919668	0.849049
14	1	0	-1.757429	3.149163	0.057549
15	8	0	-4.119947	-0.672767	0.244000
16	1	0	-3.437508	0.091619	0.354199
17	6	0	-3.958072	-1.160942	-1.076263
18	1	0	-4.646124	-2.002207	-1.213686
19	1	0	-4.197060	-0.397191	-1.831392
20	1	0	-2.933855	-1.510455	-1.263343

E(MP2) = -395.3484021
Zero-point correction = 0.165904
Sum of electronic and zero-point Energies = -395.182498
Sum of electronic and thermal Free Energies = -395.228004
One imaginary frequency of -273.4534

PC11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.349450	0.230890	-0.731903
2	8	0	1.711542	1.414509	-0.053340
3	6	0	0.834423	1.774506	1.030699
4	8	0	1.853106	-0.959005	-0.126545
5	6	0	1.057071	-1.462009	0.966902
6	53	0	-2.661518	-0.076797	-0.124566
7	1	0	0.259877	0.157519	-0.832224
8	1	0	1.850264	0.282956	-1.699249
9	1	0	0.896849	2.859905	1.127658
10	1	0	-0.196330	1.474947	0.815637
11	1	0	1.170026	1.312527	1.965085
12	1	0	1.245168	-2.535832	1.012962
13	1	0	1.370491	-0.999797	1.908468
14	1	0	-0.005308	-1.271380	0.785924
15	8	0	4.671382	-0.825720	0.196077
16	1	0	3.693490	-0.931026	0.141250
17	6	0	5.013072	0.284107	-0.633912
18	1	0	6.067647	0.502849	-0.454142
19	1	0	4.883236	0.047510	-1.698319
20	1	0	4.412696	1.166837	-0.391317

E(MP2) = -395.4236903

Zero-point correction = 0.172018
Sum of electronic and zero-point Energies = -395.251672
Sum of electronic and thermal Free Energies = -395.297703
No imaginary frequency

RC12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.640904	0.695808	-0.186354
2	8	0	0.211042	0.514994	-1.467568
3	6	0	-0.316545	-0.805577	-1.709131
4	8	0	-1.926827	-0.339765	1.123376
5	8	0	-3.422739	-1.937691	-0.297087
6	53	0	2.736029	-0.176448	0.122581
7	8	0	-1.992503	2.250168	0.657650
8	6	0	-2.615068	2.425420	-0.603704
9	6	0	-2.231950	-0.565634	2.478127
10	6	0	-4.378368	-1.087767	-0.903244
11	1	0	0.800933	1.752829	-0.002035
12	1	0	0.030481	0.183728	0.563096
13	1	0	-1.991676	1.245881	0.860340
14	1	0	-3.667007	2.106128	-0.592121
15	1	0	-2.094977	1.874762	-1.399226
16	1	0	-2.583719	3.492469	-0.846716
17	1	0	-1.474610	-0.122063	3.148806
18	1	0	-3.206416	-0.132352	2.771580
19	1	0	-2.278688	-1.643006	2.713354
20	1	0	-2.819332	-1.335473	0.279733
21	1	0	-4.892439	-0.454796	-0.166404
22	1	0	-5.124951	-1.715203	-1.401342
23	1	0	-3.927394	-0.425611	-1.657474
24	1	0	-1.028655	-1.074575	-0.927160
25	1	0	0.510710	-1.523374	-1.745638
26	1	0	-0.807428	-0.752772	-2.680738

E(MP2) = -510.7420445
Zero-point correction = 0.221035
Sum of electronic and zero-point Energies = -510.521009
Sum of electronic and thermal Free Energies = -510.574016
No imaginary frequency

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.304102	0.085306	0.291147
2	8	0	-0.056479	0.933800	-0.643751
3	6	0	-0.290303	0.329099	-1.933640
4	8	0	-1.827161	-0.472047	0.906750
5	8	0	-3.021509	-1.603926	-1.130271
6	53	0	2.934650	-0.077218	0.038656
7	8	0	-3.304925	1.727670	1.155437
8	6	0	-3.055186	2.405204	-0.067448
9	6	0	-1.790935	-1.292192	2.048658

10	6	0	-4.411636	-1.432183	-0.889173
11	1	0	0.376609	0.497090	1.282745
12	1	0	0.239598	-0.977083	0.123415
13	1	0	-2.743885	0.885488	1.130804
14	1	0	-3.253144	1.762474	-0.937095
15	1	0	-2.019791	2.761977	-0.137131
16	1	0	-3.727990	3.267046	-0.113440
17	1	0	-0.789463	-1.737089	2.205640
18	1	0	-2.039264	-0.732219	2.966339
19	1	0	-2.500427	-2.135253	1.980453
20	1	0	-2.534585	-1.204992	-0.326582
21	1	0	-4.787981	-2.144456	-0.140878
22	1	0	-4.942280	-1.611140	-1.829278
23	1	0	-4.638526	-0.417836	-0.539415
24	1	0	-1.109146	-0.388438	-1.853336
25	1	0	0.639602	-0.139696	-2.269694
26	1	0	-0.561448	1.151286	-2.593894

E(MP2) = -510.7337805
Zero-point correction = 0.221135
Sum of electronic and zero-point Energies = -510.512646
Sum of electronic and thermal Free Energies = -510.565230
One imaginary frequency of -317.3740

PC12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722996	-0.647767	0.708637
2	8	0	-1.195081	0.326361	1.585099
3	6	0	-0.496634	1.584400	1.439722
4	8	0	-1.313749	-0.422730	-0.596408
5	8	0	-2.716148	1.969373	-1.324885
6	53	0	3.089427	-0.049377	-0.045015
7	8	0	-3.842462	-1.715188	-0.397639
8	6	0	-4.095599	-1.682023	1.008024
9	6	0	-0.538689	-1.052637	-1.644066
10	6	0	-3.855334	1.931524	-0.464429
11	1	0	-1.073391	-1.614877	1.087212
12	1	0	0.368743	-0.622725	0.606242
13	1	0	-2.983018	-1.261649	-0.552289
14	1	0	-3.886780	-0.694947	1.432980
15	1	0	-3.496321	-2.427961	1.544843
16	1	0	-5.152515	-1.918317	1.146756
17	1	0	0.503049	-0.725291	-1.586469
18	1	0	-0.594799	-2.143510	-1.547978
19	1	0	-1.000665	-0.745085	-2.582782
20	1	0	-2.151543	1.200240	-1.092469
21	1	0	-4.457415	1.031691	-0.631443
22	1	0	-4.455176	2.812167	-0.702302
23	1	0	-3.563971	1.975130	0.592172
24	1	0	-0.862519	2.128519	0.565252
25	1	0	0.578934	1.409927	1.343659
26	1	0	-0.717220	2.150147	2.345759

E(MP2) = -510.7922858

Zero-point correction = 0.226629
Sum of electronic and zero-point Energies = -510.565657
Sum of electronic and thermal Free Energies = -510.617103
No imaginary frequency

RC13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.841177	0.174250	0.031268
2	8	0	-0.463734	0.119072	1.341711
3	6	0	-0.420289	-1.214864	1.876198
4	8	0	2.528200	0.335195	-1.021027
5	8	0	1.490519	-2.014107	-0.656645
6	53	0	-3.100803	-0.044515	-0.198425
7	8	0	1.129547	2.560207	-0.791451
8	6	0	1.507628	3.071715	0.481216
9	6	0	3.219006	0.339900	-2.250878
10	6	0	2.577441	-2.905205	-0.856882
11	1	0	-0.638653	1.163810	-0.368831
12	1	0	-0.465009	-0.647702	-0.578184
13	1	0	1.640817	1.690270	-0.916053
14	1	0	2.593399	3.019495	0.628272
15	1	0	1.021463	2.524083	1.300502
16	1	0	1.194307	4.119239	0.528652
17	1	0	2.617353	-0.106790	-3.060867
18	1	0	3.478597	1.363700	-2.565262
19	1	0	4.161361	-0.232237	-2.192416
20	1	0	1.857708	-1.064611	-0.814353
21	1	0	2.775433	-3.076529	-1.925851
22	1	0	2.322181	-3.866209	-0.399703
23	1	0	3.497103	-2.527009	-0.393200
24	1	0	0.198538	-1.845715	1.232887
25	1	0	-1.440071	-1.609598	1.955229
26	1	0	0.019121	-1.118919	2.868919
27	8	0	4.166962	0.218702	1.073636
28	6	0	3.280560	-0.214868	2.096326
29	1	0	3.601422	0.308764	0.238535
30	1	0	3.847267	-0.255449	3.031754
31	1	0	2.436783	0.475824	2.224704
32	1	0	2.872494	-1.213263	1.888522

E(MP2) = -626.1227991
Zero-point correction = 0.275917
Sum of electronic and zero-point Energies = -625.846882
Sum of electronic and thermal Free Energies = -625.907060
No imaginary frequency

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.485564	0.139529	-0.006544
2	8	0	-0.224281	-0.072255	1.253464
3	6	0	-0.302757	-1.455712	1.674973

4	8	0	1.614288	0.162915	-0.763231
5	8	0	1.864925	-2.503317	-0.568996
6	53	0	-3.258219	0.073253	-0.081018
7	8	0	1.690685	2.727359	0.172886
8	6	0	2.941654	3.270243	-0.236647
9	6	0	1.566247	0.396455	-2.161300
10	6	0	3.143788	-2.899959	-1.056132
11	1	0	-0.519161	1.172335	-0.310853
12	1	0	-0.569816	-0.680046	-0.702710
13	1	0	1.685818	1.763846	-0.086802
14	1	0	3.084078	3.191111	-1.323342
15	1	0	3.782042	2.773443	0.260671
16	1	0	2.936569	4.328859	0.034669
17	1	0	1.037121	1.334497	-2.394607
18	1	0	2.578239	0.471296	-2.589729
19	1	0	1.042591	-0.417168	-2.689956
20	1	0	1.809875	-1.500547	-0.628461
21	1	0	3.277271	-2.625596	-2.111327
22	1	0	3.198345	-3.988329	-0.973719
23	1	0	3.954328	-2.450240	-0.472264
24	1	0	0.356567	-2.068880	1.058566
25	1	0	-1.348084	-1.764889	1.591695
26	1	0	0.022455	-1.455170	2.713626
27	8	0	3.974169	0.048247	0.592387
28	6	0	3.445793	-0.168108	1.899530
29	1	0	3.180115	0.104746	-0.007991
30	1	0	4.267457	-0.038771	2.608748
31	1	0	2.653873	0.552751	2.134942
32	1	0	3.042673	-1.183914	2.007438

E(MP2) = -626.1079484
Zero-point correction = 0.276501
Sum of electronic and zero-point Energies = -625.831447
Sum of electronic and thermal Free Energies = -625.890238
One imaginary frequency of -333.7399

PC13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.305413	0.332840	-0.651853
2	8	0	0.716192	1.276666	0.304138
3	6	0	-0.071617	1.224592	1.518753
4	8	0	0.822406	-0.956513	-0.272763
5	8	0	2.369617	-1.494511	2.081970
6	53	0	-3.580911	0.052525	-0.121032
7	8	0	3.131801	-1.330148	-1.894485
8	6	0	4.313139	-1.341387	-1.085132
9	6	0	-0.103669	-2.044708	-0.517672
10	6	0	3.152191	-0.385496	2.529770
11	1	0	0.766778	0.634670	-1.597143
12	1	0	-0.787930	0.285718	-0.720091
13	1	0	2.359754	-1.233826	-1.294286
14	1	0	4.268066	-2.125468	-0.321242
15	1	0	4.473723	-0.374038	-0.597597
16	1	0	5.147800	-1.547624	-1.757832
17	1	0	-1.092631	-1.793147	-0.124146

18	1	0	-0.174368	-2.243551	-1.592002
19	1	0	0.320079	-2.911089	-0.009686
20	1	0	1.833962	-1.206088	1.311776
21	1	0	3.814589	-0.005617	1.745871
22	1	0	3.752122	-0.747218	3.366268
23	1	0	2.521226	0.440001	2.882232
24	1	0	0.158227	0.316111	2.082486
25	1	0	-1.136132	1.245934	1.271511
26	1	0	0.219349	2.104328	2.093367
27	8	0	3.429645	2.029459	0.028286
28	6	0	3.489299	2.377825	-1.356903
29	1	0	2.502487	1.766613	0.222785
30	1	0	4.490778	2.772059	-1.538408
31	1	0	3.329203	1.504331	-1.999401
32	1	0	2.755387	3.152433	-1.608724

E(MP2) = -626.1631696
Zero-point correction = 0.281260
Sum of electronic and zero-point Energies = -625.881909
Sum of electronic and thermal Free Energies = -625.941087
No imaginary frequency

RC21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.383867	-0.392232	-0.073777
2	53	0	-1.808958	-0.190763	0.026619
3	8	0	1.010163	0.700306	-0.657228
4	6	0	1.036675	1.866697	0.185139
5	8	0	3.482558	-0.301369	0.386792
6	6	0	4.778778	-0.698986	-0.071935
7	1	0	0.705900	-0.562522	0.955862
8	1	0	0.557399	-1.257690	-0.707577
9	1	0	1.511997	1.627720	1.141707
10	1	0	1.624914	2.607815	-0.353181
11	1	0	0.019510	2.235481	0.343926
12	1	0	2.957401	0.040508	-0.361308
13	1	0	5.309947	-1.064998	0.805731
14	1	0	4.716633	-1.504166	-0.811598
15	1	0	5.333369	0.143918	-0.497469

E(MP2) = -280.552017
Zero-point correction = 0.126511
Sum of electronic and zero-point Energies = -280.425506
Sum of electronic and thermal Free Energies = -280.466108
No imaginary frequency

TS21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.482414	0.702304	1.021416
2	8	0	-1.817038	1.769160	0.425919

3	6	0	-1.393560	1.910939	-0.989613
4	8	0	-2.939691	-0.895194	0.097886
5	6	0	-2.298735	-2.106406	-0.387160
6	53	0	1.620112	-0.155529	0.005895
7	1	0	-0.771600	0.003037	0.580000
8	1	0	-1.808817	0.643391	2.055763
9	1	0	-1.405895	2.982028	-1.167617
10	1	0	-0.397387	1.470675	-1.085064
11	1	0	-2.145445	1.390370	-1.579277
12	1	0	-3.857966	-1.100997	0.350373
13	1	0	-2.794860	-2.453935	-1.295925
14	1	0	-1.265401	-1.838739	-0.606936
15	1	0	-2.316505	-2.885547	0.377926

E(MP2) = -280.4918414
Zero-point correction = 0.125559
Sum of electronic and zero-point Energies = -280.366282
Sum of electronic and thermal Free Energies = -280.404258
One imaginary frequency of -125.7084

PC21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.582757	0.230663	0.621954
2	8	0	-2.377003	-1.140715	0.626268
3	6	0	-2.651757	-1.754826	-0.641652
4	8	0	-1.623489	0.841627	-0.244154
5	6	0	-1.761426	2.266340	-0.280316
6	1	0	-3.593711	0.490510	0.262414
7	1	0	-2.438421	0.577465	1.650942
8	1	0	-3.666966	-1.504940	-0.973473
9	1	0	-1.927469	-1.437374	-1.394990
10	1	0	-2.571589	-2.827722	-0.475017
11	1	0	0.152283	0.220439	-0.047431
12	1	0	-0.981989	2.632640	-0.946819
13	1	0	-2.745520	2.548278	-0.672055
14	1	0	-1.625374	2.696761	0.718732
15	53	0	1.761855	-0.102951	0.011714

E(MP2) = -280.5488147
Zero-point correction = 0.123513
Sum of electronic and zero-point Energies = -280.425302
Sum of electronic and thermal Free Energies = -280.464441
No imaginary frequency

RC22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.720949	1.318958	-0.881601
2	8	0	-1.105249	2.388581	-0.125426
3	6	0	-0.364619	2.535793	1.100710
4	8	0	2.459415	0.990701	-0.214673

5	6	0	3.836500	1.325700	-0.409856
6	53	0	-1.482698	-0.644687	-0.053316
7	8	0	1.971087	-1.562864	0.838365
8	6	0	2.294213	-2.646531	-0.050718
9	1	0	0.358855	1.166428	-0.926108
10	1	0	-1.213211	1.372818	-1.848645
11	1	0	0.706476	2.435048	0.908645
12	1	0	-0.607065	3.529551	1.473093
13	1	0	-0.692631	1.776089	1.817668
14	1	0	2.405833	0.099613	0.202696
15	1	0	0.996642	-1.486267	0.880136
16	1	0	1.913216	-3.594775	0.337599
17	1	0	3.381695	-2.687372	-0.096559
18	1	0	1.892066	-2.469270	-1.052672
19	1	0	4.334667	0.610848	-1.074149
20	1	0	3.856482	2.311418	-0.874867
21	1	0	4.377054	1.369438	0.541588

E(MP2) = -395.9215775
Zero-point correction = 0.181522
Sum of electronic and zero-point Energies = -395.740055
Sum of electronic and thermal Free Energies = -395.787396
No imaginary frequency

TS22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156558	-0.699459	0.560589
2	8	0	1.549114	-1.905542	0.822224
3	6	0	1.635906	-2.806046	-0.323395
4	8	0	2.682696	0.550921	0.408558
5	6	0	3.563053	0.397689	-0.724675
6	53	0	-1.859230	-0.276967	-0.080754
7	8	0	0.618314	2.160757	-0.134130
8	6	0	0.220151	3.501540	0.205579
9	1	0	0.838204	-0.455185	-0.442002
10	1	0	0.833293	-0.127465	1.416096
11	1	0	2.453606	-2.490452	-0.971866
12	1	0	1.836679	-3.785960	0.100583
13	1	0	0.675750	-2.788627	-0.841578
14	1	0	2.071386	1.331685	0.244048
15	1	0	-0.200374	1.592965	-0.185582
16	1	0	-0.437336	3.906746	-0.566678
17	1	0	1.131627	4.096855	0.257267
18	1	0	-0.288587	3.521551	1.172460
19	1	0	4.204046	1.277510	-0.805977
20	1	0	4.174507	-0.482354	-0.529009
21	1	0	2.991391	0.270520	-1.649612

E(MP2) = -395.8793587
Zero-point correction = 0.182137
Sum of electronic and zero-point Energies = -395.697222
Sum of electronic and thermal Free Energies = -395.741555
One imaginary frequency of -229.7487

PC22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.090736	0.213688	-0.683683
2	8	0	-3.395114	-0.286239	-0.617295
3	6	0	-3.475819	-1.709292	-0.431262
4	8	0	-1.824489	1.094421	0.423128
5	6	0	-1.913213	0.430343	1.706970
6	53	0	1.754942	-0.777921	0.003234
7	8	0	0.571026	2.100114	0.358489
8	6	0	0.866413	2.883754	-0.839212
9	1	0	-1.343119	-0.589740	-0.688669
10	1	0	-1.994071	0.853271	-1.563276
11	1	0	-3.048642	-2.238039	-1.288454
12	1	0	-2.961933	-2.021430	0.483232
13	1	0	-4.537906	-1.936562	-0.353616
14	1	0	-0.408215	1.789004	0.352079
15	1	0	1.112171	1.120114	0.304037
16	1	0	1.905136	3.191925	-0.751941
17	1	0	0.201439	3.744992	-0.832635
18	1	0	0.721554	2.268926	-1.728505
19	1	0	-1.622623	1.172794	2.449733
20	1	0	-2.943038	0.116606	1.880403
21	1	0	-1.223923	-0.419385	1.734766

E(MP2) = -395.9163999
Zero-point correction = 0.181306
Sum of electronic and zero-point Energies = -395.735094
Sum of electronic and thermal Free Energies = -395.778177
No imaginary frequency

RC23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.473697	1.045133	-0.826890
2	8	0	-0.742570	2.314754	-0.401223
3	6	0	-0.539591	2.517465	1.010406
4	8	0	2.588222	1.324961	0.651008
5	6	0	3.021914	2.452225	-0.114997
6	8	0	2.543922	-1.006074	-0.857191
7	6	0	3.543658	-1.844290	-1.452243
8	8	0	0.879290	-2.206513	0.980492
9	6	0	1.144057	-1.599544	2.262047
10	53	0	-2.074180	-0.432918	-0.236843
11	1	0	-0.045733	-2.009001	0.729870
12	1	0	0.434800	0.615356	-0.402040
13	1	0	-0.503596	1.017324	-1.912632
14	1	0	2.744895	0.514384	0.112864
15	1	0	4.097769	2.412194	-0.317734
16	1	0	2.479348	2.526625	-1.064908
17	1	0	2.810503	3.340953	0.480646
18	1	0	-0.620462	3.592081	1.165335
19	1	0	0.449073	2.152812	1.301321
20	1	0	-1.325956	1.999686	1.569398

21	1	0	1.063880	-0.510254	2.207894
22	1	0	2.167586	-1.870030	2.517424
23	1	0	0.463207	-1.992785	3.021236
24	1	0	1.971986	-1.553150	-0.264136
25	1	0	4.197062	-2.285213	-0.692795
26	1	0	3.082147	-2.640454	-2.043520
27	1	0	4.136094	-1.208820	-2.110161

E(MP2) = -511.2912368
Zero-point correction = 0.236353
Sum of electronic and zero-point Energies = -511.054884
Sum of electronic and thermal Free Energies = -511.109282
No imaginary frequency

TS23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.809277	-1.106917	0.018364
2	8	0	-0.660115	-2.375309	0.252029
3	6	0	-0.252103	-2.703006	1.610628
4	8	0	-2.712545	-0.787562	0.383669
5	6	0	-3.588370	-1.530484	-0.487603
6	8	0	-2.455916	1.789317	-0.186491
7	6	0	-2.359179	2.265715	-1.541048
8	8	0	-0.053064	2.025989	1.029697
9	6	0	0.541450	3.011913	1.889239
10	53	0	2.036295	-0.203218	-0.487966
11	1	0	0.670747	1.530159	0.559900
12	1	0	-0.569889	-0.373442	0.774755
13	1	0	-0.888716	-0.836716	-1.024203
14	1	0	-2.774484	0.199269	0.176469
15	1	0	-4.625550	-1.313574	-0.225321
16	1	0	-3.404712	-1.277447	-1.536825
17	1	0	-3.376218	-2.586164	-0.321925
18	1	0	-0.226480	-3.788688	1.650099
19	1	0	-0.986103	-2.302134	2.311645
20	1	0	0.740470	-2.276487	1.766808
21	1	0	1.225341	2.537379	2.597343
22	1	0	-0.275010	3.486863	2.433182
23	1	0	1.080228	3.763688	1.306398
24	1	0	-1.605025	2.009522	0.280753
25	1	0	-2.275233	3.355069	-1.553499
26	1	0	-1.496649	1.828390	-2.053761
27	1	0	-3.278356	1.972057	-2.048335

E(MP2) = -511.2630145
Zero-point correction = 0.236958
Sum of electronic and zero-point Energies = -511.026057
Sum of electronic and thermal Free Energies = -511.077508
One imaginary frequency of -290.0577

PC23

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.243555	-0.375031	-0.704231
2	8	0	3.520788	-0.924675	-0.863901
3	6	0	4.546815	0.071602	-0.951309
4	8	0	2.102078	0.305503	0.546054
5	6	0	2.113014	-0.607312	1.666357
6	8	0	0.290924	2.327059	0.591579
7	6	0	-0.390009	2.315024	1.870749
8	8	0	-1.184973	1.586789	-1.312673
9	6	0	-2.466180	2.283487	-1.384219
10	53	0	-1.652196	-1.219361	0.061678
11	1	0	-1.355032	0.571728	-0.978037
12	1	0	2.039527	0.389389	-1.465017
13	1	0	1.531425	-1.200909	-0.764907
14	1	0	0.979605	1.603139	0.601586
15	1	0	2.024304	0.009331	2.560968
16	1	0	1.263550	-1.291703	1.591560
17	1	0	3.055831	-1.157783	1.686823
18	1	0	5.471425	-0.465664	-1.157841
19	1	0	4.638637	0.626493	-0.013368
20	1	0	4.333846	0.769796	-1.770132
21	1	0	-3.004473	1.859053	-2.228145
22	1	0	-2.246539	3.335861	-1.552460
23	1	0	-3.021805	2.131006	-0.458033
24	1	0	-0.581747	1.973993	-0.531377
25	1	0	-1.107872	3.134614	1.850729
26	1	0	-0.903814	1.362021	2.019392
27	1	0	0.335791	2.491739	2.666790

E(MP2) = -511.2974512
Zero-point correction = 0.237015
Sum of electronic and zero-point Energies = -511.060436
Sum of electronic and thermal Free Energies = -511.109747
No imaginary frequency

RC24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.634327	-0.917415	-0.681447
2	8	0	3.369011	0.021037	0.852773
3	8	0	1.649697	2.192509	1.212133
4	8	0	0.094809	2.393629	-1.067342
5	8	0	-2.549403	1.778755	-0.588544
6	53	0	-1.373121	-1.585359	0.154782
7	6	0	4.161758	0.294854	-0.304225
8	6	0	0.755721	2.055218	2.323516
9	6	0	0.274800	3.476830	-1.992544
10	6	0	-3.190840	2.302481	0.588188
11	1	0	2.850069	0.834515	1.055818
12	1	0	1.108375	2.310473	0.392970
13	1	0	-0.872812	2.249546	-0.920510
14	1	0	-2.517959	0.802773	-0.514768
15	1	0	4.692353	-0.625502	-0.551443
16	1	0	4.894658	1.086257	-0.112510
17	1	0	3.539286	0.581996	-1.160880

18	1	0	0.099450	1.185212	2.204548
19	1	0	1.373343	1.915270	3.210636
20	1	0	0.147740	2.957040	2.450699
21	1	0	1.348276	3.578981	-2.150229
22	1	0	-0.119979	4.414221	-1.588629
23	1	0	-0.211197	3.254816	-2.946651
24	1	0	-4.229322	1.966424	0.643143
25	1	0	-2.656130	2.004882	1.494926
26	1	0	-3.167337	3.387026	0.490116
27	8	0	1.328440	-1.944831	-1.242018
28	1	0	0.354798	-0.196225	-1.443475
29	1	0	1.119682	-0.477615	0.188954
30	6	0	1.956653	-2.817002	-0.281091
31	1	0	1.188622	-3.400556	0.237246
32	1	0	2.597234	-3.478467	-0.861765
33	1	0	2.541330	-2.225617	0.427979

E(MP2) = -626.660567
Zero-point correction = 0.291106
Sum of electronic and zero-point Energies = -626.369461
Sum of electronic and thermal Free Energies = -626.433653
No imaginary frequency

TS24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.666498	-1.385641	-0.173976
2	8	0	2.551977	-1.596224	0.444988
3	8	0	2.526095	0.783248	1.623857
4	8	0	1.671577	1.785886	-0.743491
5	8	0	-0.886069	2.566284	-0.967730
6	53	0	-2.185914	-0.425718	0.131946
7	6	0	3.478672	-1.537361	-0.659298
8	6	0	1.578570	1.021486	2.684261
9	6	0	2.470280	2.596090	-1.620854
10	6	0	-1.412571	3.540459	-0.051936
11	1	0	2.652040	-0.755178	0.993297
12	1	0	2.241894	1.303237	0.826059
13	1	0	0.722739	2.101090	-0.805979
14	1	0	-1.387025	1.722383	-0.826631
15	1	0	3.251989	-2.382640	-1.308188
16	1	0	4.498533	-1.623956	-0.279142
17	1	0	3.357667	-0.601834	-1.213829
18	1	0	0.556824	0.797572	2.360027
19	1	0	1.855405	0.363098	3.507213
20	1	0	1.640029	2.060442	3.018242
21	1	0	3.497516	2.237182	-1.542681
22	1	0	2.436086	3.648944	-1.325457
23	1	0	2.126599	2.495505	-2.653736
24	1	0	-2.456285	3.760399	-0.288859
25	1	0	-1.340771	3.188337	0.981411
26	1	0	-0.813803	4.443012	-0.177089
27	8	0	0.529230	-2.342565	-1.038719
28	1	0	0.860303	-0.405127	-0.587445
29	1	0	0.351247	-1.523908	0.849293
30	6	0	0.034540	-3.599319	-0.496072

31	1	0	-0.973606	-3.420161	-0.117599
32	1	0	0.025008	-4.291521	-1.333768
33	1	0	0.712652	-3.941120	0.287738

E(MP2) = -626.6379774
Zero-point correction = 0.292257
Sum of electronic and zero-point Energies = -626.345720
Sum of electronic and thermal Free Energies = -626.403384
One imaginary frequency of -279.6593

PC24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.431881	-0.201105	1.268400
2	8	0	-2.345069	1.054210	0.581488
3	8	0	-0.532861	2.056422	-1.153927
4	8	0	1.747590	2.279955	-0.111630
5	8	0	1.712359	0.753125	1.869735
6	53	0	1.018129	-1.547558	-0.397248
7	6	0	-3.481559	1.901340	0.819052
8	6	0	-0.651949	1.426997	-2.453310
9	6	0	2.802066	1.891598	-1.050072
10	6	0	2.933952	0.468308	2.585060
11	1	0	-1.138184	1.587979	-0.516777
12	1	0	0.792392	2.149944	-0.562226
13	1	0	1.773983	1.656770	0.761235
14	1	0	1.422095	-0.080926	1.382814
15	1	0	-4.392752	1.442492	0.429243
16	1	0	-3.277855	2.839354	0.302091
17	1	0	-3.591901	2.084863	1.893385
18	1	0	-0.289647	0.398485	-2.408487
19	1	0	-1.696681	1.458956	-2.769304
20	1	0	-0.050056	2.019580	-3.142352
21	1	0	2.694629	2.533204	-1.922846
22	1	0	2.691134	0.836211	-1.301773
23	1	0	3.750701	2.088836	-0.554109
24	1	0	2.717685	-0.212114	3.409822
25	1	0	3.675503	0.018817	1.919358
26	1	0	3.299579	1.417467	2.975639
27	8	0	-3.515964	-0.970987	0.834281
28	1	0	-2.597172	-0.015129	2.334294
29	1	0	-1.474502	-0.691754	1.073698
30	6	0	-3.324726	-1.489958	-0.493249
31	1	0	-2.358103	-1.996895	-0.570163
32	1	0	-4.139215	-2.194099	-0.658954
33	1	0	-3.376336	-0.686331	-1.235306

E(MP2) = -626.6720863
Zero-point correction = 0.292792
Sum of electronic and zero-point Energies = -626.379295
Sum of electronic and thermal Free Energies = -626.435235
No imaginary frequency

RC23'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.546508	0.173002	0.032513
2	8	0	0.034570	-1.032725	-0.393728
3	6	0	0.175072	-2.091228	0.563246
4	8	0	-2.374332	-0.128374	1.494904
5	6	0	-3.390242	-0.243268	2.501725
6	53	0	2.769822	0.234061	-0.000540
7	8	0	-3.187188	-0.909198	-1.027117
8	6	0	-2.722417	-1.854581	-2.003290
9	8	0	-2.195183	1.687207	-0.623472
10	6	0	-2.971319	2.891968	-0.683558
11	1	0	0.283595	0.405975	1.066951
12	1	0	0.236435	0.946561	-0.663324
13	1	0	-0.242091	-1.782179	1.526581
14	1	0	-0.387219	-2.933742	0.161569
15	1	0	1.230002	-2.363110	0.671962
16	1	0	-3.452945	-1.268305	2.879609
17	1	0	-3.101132	0.419946	3.316637
18	1	0	-4.369047	0.060200	2.116344
19	1	0	-2.835753	-0.016459	-1.247299
20	1	0	-3.127778	-1.620572	-2.992422
21	1	0	-1.630244	-1.869622	-2.040413
22	1	0	-3.096523	-2.829811	-1.691350
23	1	0	-2.224510	1.325873	0.292865
24	1	0	-4.018618	2.705510	-0.423269
25	1	0	-2.560397	3.658321	-0.019425
26	1	0	-2.916170	3.245561	-1.712419
27	1	0	-2.636697	-0.680010	0.717516

E(MP2) = -511.2923257
Zero-point correction = 0.236938
Sum of electronic and zero-point Energies = -511.055388
Sum of electronic and thermal Free Energies = -511.108199
No imaginary frequency

RC24'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.608396	-0.441616	-0.380242
2	8	0	0.492789	-1.756027	-0.771186
3	6	0	0.709147	-2.696373	0.291923
4	8	0	-2.078618	-0.849868	1.620218
5	6	0	-3.077807	-1.300493	2.548318
6	53	0	2.719020	0.206173	-0.084189
7	8	0	-2.972731	-0.935944	-0.948965
8	6	0	-2.694019	-1.935577	-1.943374
9	8	0	-1.874973	1.549669	-1.415603
10	6	0	-2.605696	2.594251	-2.075624
11	8	0	-1.692494	1.865459	1.299579
12	6	0	-0.594552	2.419767	2.040630
13	1	0	0.137369	-0.241350	0.583533
14	1	0	0.236174	0.199534	-1.174785
15	1	0	0.048954	-2.466869	1.134263

16	1	0	0.471854	-3.674661	-0.123785
17	1	0	1.756785	-2.668088	0.608706
18	1	0	-3.234795	-2.379226	2.455854
19	1	0	-2.705009	-1.077580	3.548066
20	1	0	-4.027025	-0.779344	2.390228
21	1	0	-2.620979	-0.062106	-1.256999
22	1	0	-3.190539	-1.686682	-2.886119
23	1	0	-1.617998	-2.044395	-2.100305
24	1	0	-3.103684	-2.873070	-1.566186
25	1	0	-1.823096	0.918103	1.559037
26	1	0	-0.515933	3.466550	1.748150
27	1	0	-0.785850	2.362528	3.116168
28	1	0	0.345939	1.911033	1.806750
29	1	0	-1.764846	1.794079	-0.460249
30	1	0	-3.597175	2.724758	-1.630885
31	1	0	-2.056852	3.539255	-2.030352
32	1	0	-2.713549	2.294042	-3.117730
33	1	0	-2.412409	-1.009763	0.696540

E(MP2) = -626.6712358
Zero-point correction = 0.292596
Sum of electronic and zero-point Energies = -626.378640
Sum of electronic and thermal Free Energies = -626.437819
No imaginary frequency