Intramolecular Cyclization Reactions of Arylpropargyl Amides of Electron-deficient α,β-Alkenyl Carboxylates and Related Compounds

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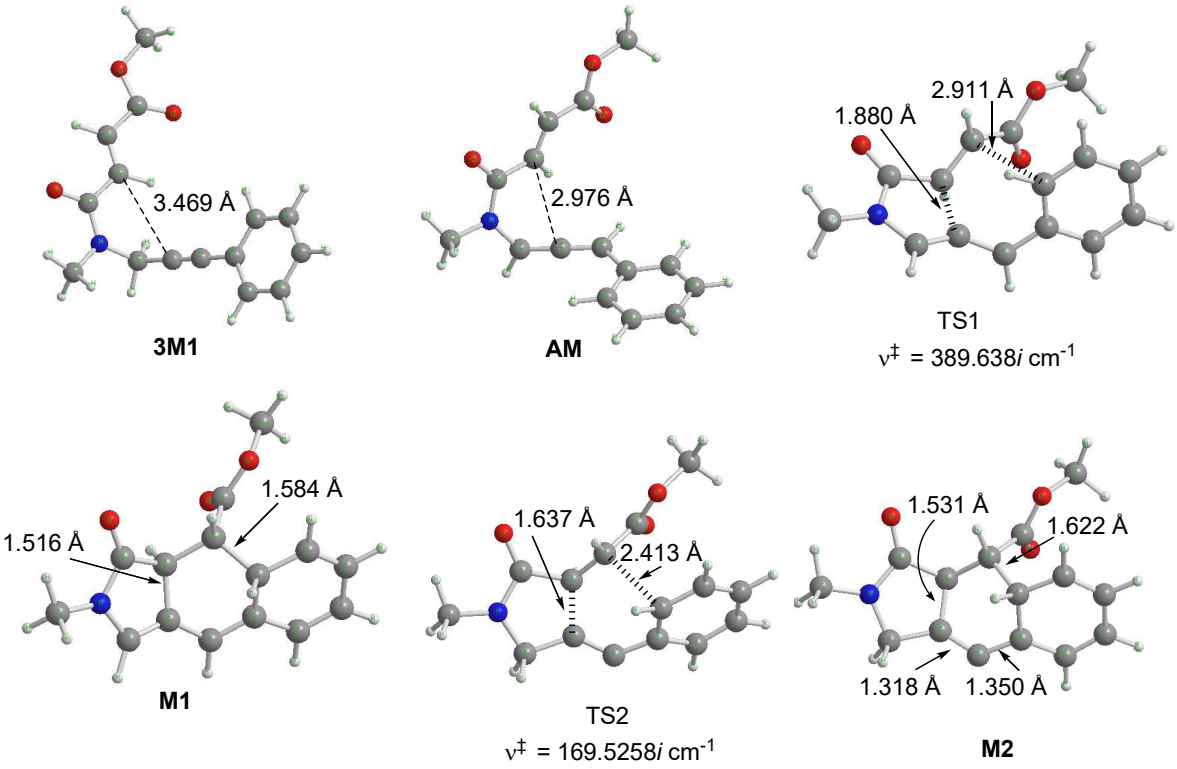
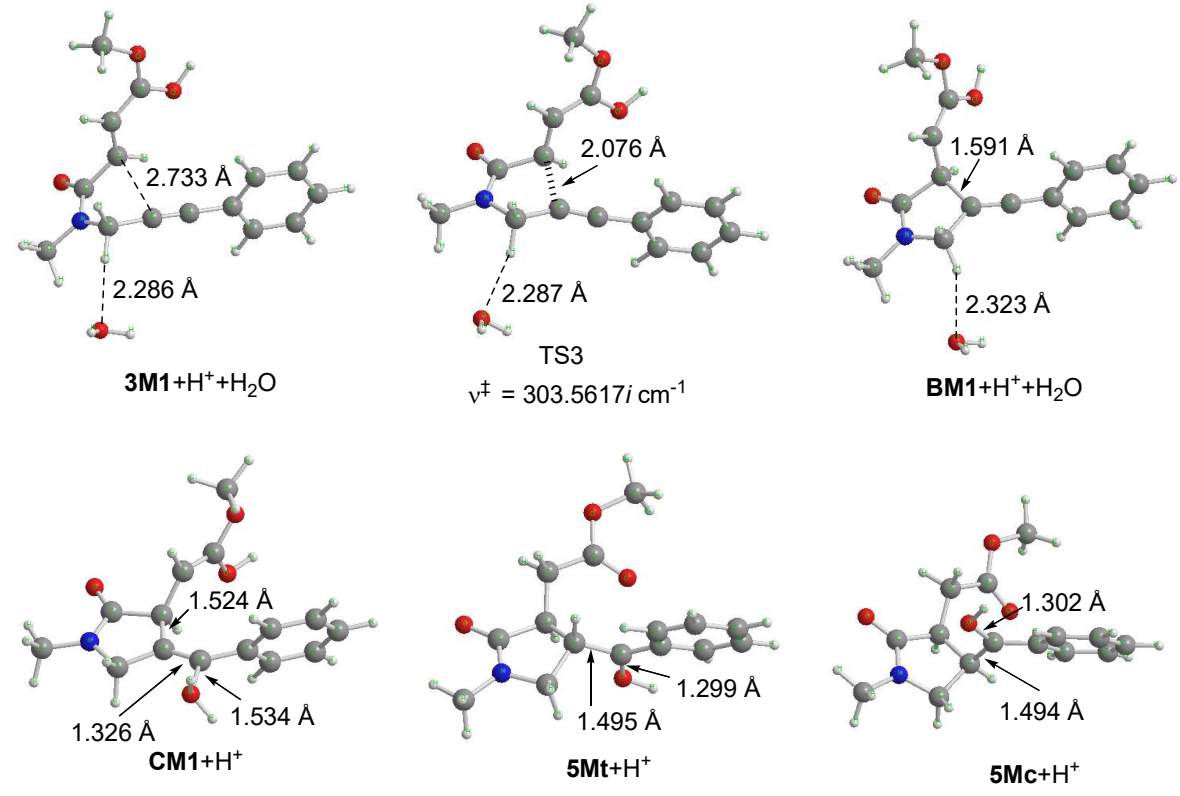
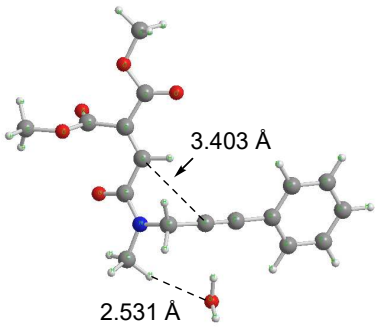
I-1. Figure S1. Optimized structures in Scheme 12.



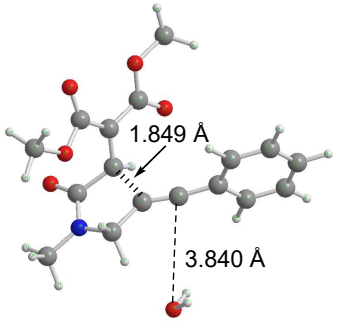
I-2. Figure S2. Optimized structures in Scheme 13.



I-3. Figure S3. Optimized structures in Scheme 14

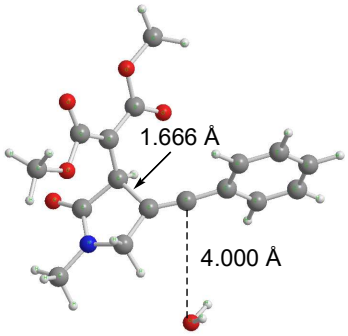


6M1+H_2O

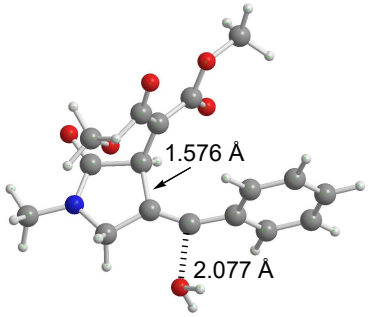


TS4

$\nu^{\ddagger}$ = 283.2513*i* cm^{-1}

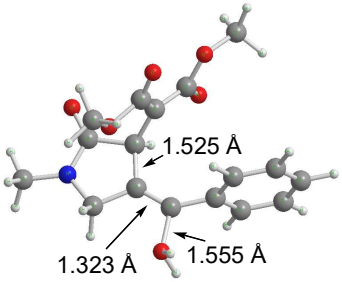


BM2+H_2O

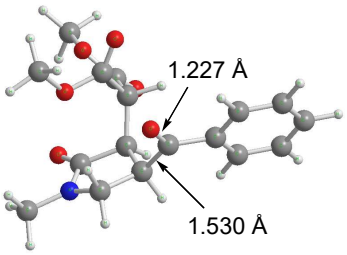


TS5

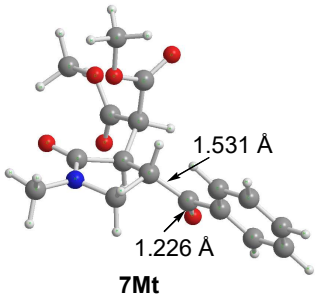
$\nu^{\ddagger}$ = 156.0821*i* cm^{-1}



CM2

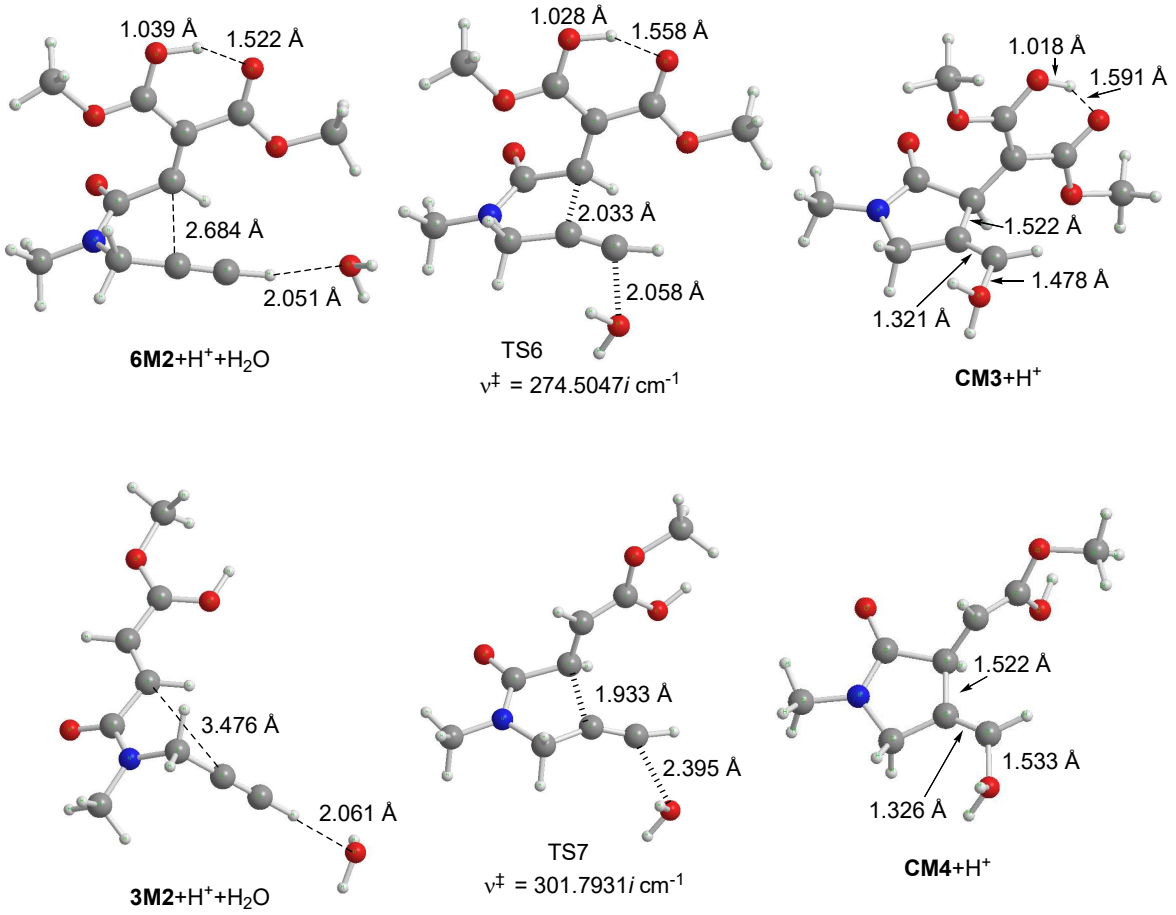


7Mc

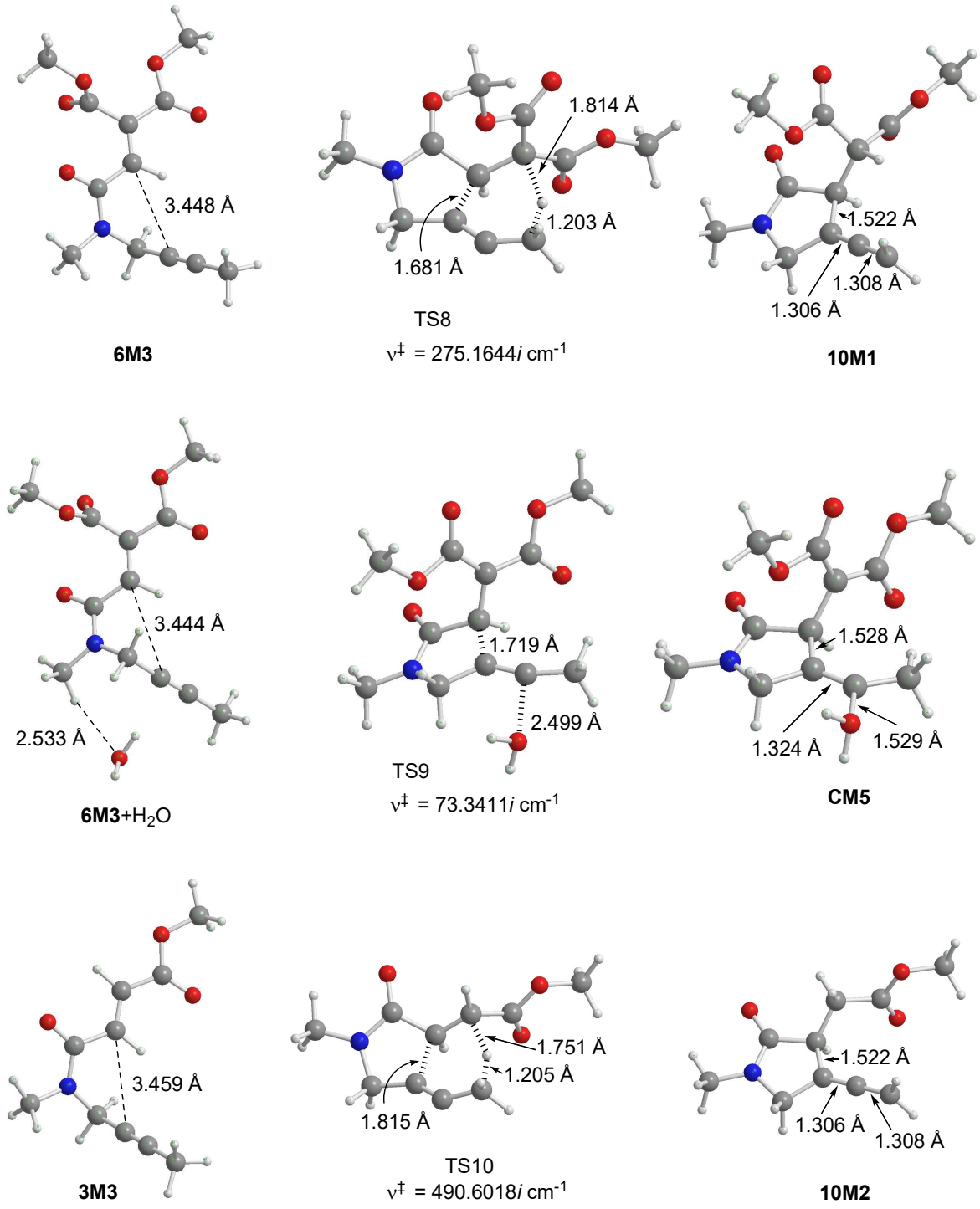


7Mt

I-4. Figure S4. Optimized structures in Scheme 15



I-5. Figure S5. Optimized structures in Scheme 16



I-6. Cartesian coordinates of the optimized geometries

Scheme 12
3M1 PhCCTS6pcm.for3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.912434	-0.542603	-0.941143
2	6	0	3.209993	-0.021359	-0.299606
3	6	0	2.055996	-0.594247	0.062588
4	1	0	1.367917	-0.032288	0.685067
5	6	0	3.553954	1.347386	0.156996
6	6	0	1.705582	-1.961780	-0.437644
7	8	0	2.348795	-2.479626	-1.352473
8	7	0	0.640581	-2.594380	0.155634
9	6	0	-0.115035	-2.057549	1.294526
10	1	0	-0.473666	-2.916204	1.875032
11	6	0	-1.250506	-1.209178	0.910963
12	6	0	-2.174470	-0.496002	0.580474
13	6	0	-3.262044	0.348814	0.194860
14	1	0	0.560393	-1.513404	1.961051
15	8	0	2.868116	2.047302	0.879296
16	8	0	4.749300	1.727636	-0.340358
17	6	0	5.185970	3.046169	0.032302
18	1	0	6.154951	3.179632	-0.448337
19	1	0	5.280689	3.124653	1.118417
20	1	0	4.474862	3.797715	-0.320319
21	6	0	0.148701	-3.846726	-0.407597
22	1	0	0.245213	-4.661677	0.320412
23	1	0	0.738583	-4.081312	-1.291727
24	1	0	-0.907323	-3.744294	-0.684126
25	6	0	-4.585988	-0.130508	0.224261
26	6	0	-5.641214	0.697554	-0.150910
27	6	0	-5.394519	2.010498	-0.560476
28	6	0	-4.084116	2.494487	-0.593189
29	6	0	-3.022950	1.673663	-0.218881
30	1	0	-4.774037	-1.151362	0.542524
31	1	0	-6.658651	0.317288	-0.124093
32	1	0	-6.219926	2.653693	-0.852746
33	1	0	-3.887778	3.514718	-0.910953
34	1	0	-2.003541	2.046283	-0.242213

SCF Done: E(RB3LYP) = -860.994426995 A.U. after 1 cycles
Zero-point correction= 0.271403 (Hartree/Particle)
Thermal correction to Energy= 0.290628
Thermal correction to Enthalpy= 0.291572
Thermal correction to Gibbs Free Energy= 0.218696
Sum of electronic and zero-point Energies= -860.723024
Sum of electronic and thermal Energies= -860.703799
Sum of electronic and thermal Enthalpies= -860.702855
Sum of electronic and thermal Free Energies= -860.775731
SCF Done: E(RB3LYP) = -861.255694412 A.U. after 15 cycles

AM PhCCTS4pcm.for.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.997396	-0.129256	-1.503917
2	6	0	2.669752	0.101405	-0.495750
3	6	0	1.930829	-0.765452	0.207969
4	1	0	1.622919	-0.510038	1.215329
5	6	0	3.061234	1.405653	0.088582
6	6	0	1.570349	-2.094872	-0.362971
7	8	0	2.176421	-2.574018	-1.320439
8	7	0	0.572064	-2.805541	0.279738
9	6	0	-0.392467	-2.242578	1.155405
10	1	0	-0.716421	-2.927138	1.940155
11	6	0	-0.902369	-1.034753	1.076890

12	6	0	-1.387783	0.187389	1.058582
13	6	0	-2.628937	0.630031	0.396505
14	1	0	-0.823277	0.969834	1.571329
15	8	0	2.732430	1.819286	1.186044
16	8	0	3.843517	2.096536	-0.767575
17	6	0	4.287323	3.382722	-0.302949
18	1	0	4.898163	3.789678	-1.108642
19	1	0	4.877439	3.276386	0.611017
20	1	0	3.431879	4.033217	-0.102738
21	6	0	0.342521	-4.187777	-0.143497
22	1	0	-0.066476	-4.751444	0.699897
23	1	0	1.288552	-4.625098	-0.460903
24	1	0	-0.366255	-4.236660	-0.978843
25	6	0	-3.460183	-0.258016	-0.308679
26	6	0	-4.623489	0.197780	-0.921085
27	6	0	-4.980601	1.548402	-0.841904
28	6	0	-4.163393	2.439012	-0.144220
29	6	0	-2.996941	1.983098	0.469875
30	1	0	-3.183686	-1.307055	-0.371512
31	1	0	-5.255456	-0.500532	-1.463332
32	1	0	-5.889395	1.901432	-1.321457
33	1	0	-4.432475	3.489691	-0.077517
34	1	0	-2.361359	2.679073	1.012217

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SCF Done:  E(RB3LYP) =  -861.000464082     A.U. after    1 cycles
Zero-point correction=                           0.270711 (Hartree/Particle)
 Thermal correction to Energy=                    0.289617
 Thermal correction to Enthalpy=                  0.290561
 Thermal correction to Gibbs Free Energy=         0.219991
 Sum of electronic and zero-point Energies=           -860.729753
 Sum of electronic and thermal Energies=              -860.710847
 Sum of electronic and thermal Enthalpies=            -860.709903
 Sum of electronic and thermal Free Energies=         -860.780473
SCF Done:  E(RB3LYP) =  -861.259533173     A.U. after   15 cycles
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TS1 PhCCTS4pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.476137	1.415735	-1.394588
2	6	0	0.370184	1.242778	-0.330136
3	6	0	1.379576	0.630407	0.427903
4	1	0	1.280578	0.820177	1.499058
5	6	0	-0.817080	1.732772	0.346483
6	6	0	2.829733	0.749060	-0.038243
7	8	0	3.392980	1.807937	-0.268907
8	7	0	3.426508	-0.488453	-0.117960
9	6	0	2.553527	-1.550036	0.148191
10	1	0	2.915827	-2.552043	-0.058493
11	6	0	1.310612	-1.245949	0.522800
12	6	0	0.139999	-1.813054	0.975830
13	6	0	-1.104936	-1.656393	0.294291
14	1	0	0.106759	-2.246445	1.977078
15	8	0	-1.043547	1.619098	1.546904
16	8	0	-1.669392	2.363359	-0.508275
17	6	0	-2.857670	2.889979	0.094676
18	1	0	-3.425235	3.342565	-0.719801
19	1	0	-2.610948	3.643538	0.848437
20	1	0	-3.438574	2.093641	0.567828
21	6	0	4.804503	-0.670040	-0.541869
22	1	0	5.399130	-1.132853	0.253032
23	1	0	5.210018	0.316748	-0.766978
24	1	0	4.855136	-1.297959	-1.438580
25	6	0	-1.156532	-1.136296	-1.025200
26	6	0	-2.387549	-0.921986	-1.654067
27	6	0	-3.572250	-1.227848	-0.993505
28	6	0	-3.538552	-1.767617	0.307577
29	6	0	-2.329143	-1.977825	0.941289
30	1	0	-0.233216	-0.995882	-1.572602
31	1	0	-2.412656	-0.526258	-2.665277
32	1	0	-4.527473	-1.066710	-1.485656
33	1	0	-4.467524	-2.012457	0.814949

34	1	0	-2.300372	-2.373481	1.953405

SCF Done: E(RB3LYP) = -860.969728322 A.U. after 1 cycles
Zero-point correction= 0.269576 (Hartree/Particle)
Thermal correction to Energy= 0.287342
Thermal correction to Enthalpy= 0.288286
Thermal correction to Gibbs Free Energy= 0.222691
Sum of electronic and zero-point Energies= -860.700153
Sum of electronic and thermal Energies= -860.682386
Sum of electronic and thermal Enthalpies= -860.681442
Sum of electronic and thermal Free Energies= -860.747037
SCF Done: E(RB3LYP) = -861.228970358 A.U. after 17 cycles

M1 PhCCTS4pcm.rev.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.099332	1.184691	-1.320206
2	6	0	-0.129653	0.627398	-0.406801
3	6	0	1.168999	0.258406	0.334674
4	1	0	1.090698	0.686762	1.345856
5	6	0	-1.000658	1.524878	0.465875
6	6	0	2.492251	0.788704	-0.218272
7	8	0	2.735531	1.893258	-0.680524
8	7	0	3.407268	-0.240388	-0.044548
9	6	0	2.756281	-1.423275	0.354986
10	1	0	3.329573	-2.338930	0.432236
11	6	0	1.432089	-1.221853	0.532586
12	6	0	0.317177	-2.087237	0.809895
13	6	0	-0.883165	-1.780015	0.240602
14	1	0	0.422827	-2.958326	1.453535
15	8	0	-1.037043	1.502615	1.679560
16	8	0	-1.751630	2.353369	-0.284255
17	6	0	-2.664312	3.197616	0.442538
18	1	0	-3.171653	3.796641	-0.313541
19	1	0	-2.117434	3.838438	1.138230
20	1	0	-3.382697	2.590431	0.998790
21	6	0	4.802611	-0.144291	-0.428655
22	1	0	5.457132	-0.348551	0.425583
23	1	0	4.974753	0.874568	-0.779350
24	1	0	5.039504	-0.847675	-1.235613
25	6	0	-0.915377	-0.681012	-0.829536
26	6	0	-2.294271	-0.395180	-1.369855
27	6	0	-3.370992	-1.121408	-1.019904
28	6	0	-3.273693	-2.215417	-0.064030
29	6	0	-2.092247	-2.518300	0.526638
30	1	0	-0.314420	-1.061631	-1.673537
31	1	0	-2.382965	0.418854	-2.083789
32	1	0	-4.342001	-0.899617	-1.456137
33	1	0	-4.169993	-2.778879	0.179951
34	1	0	-2.028628	-3.322090	1.257135

SCF Done: E(RB3LYP) = -861.021504772 A.U. after 1 cycles
Zero-point correction= 0.274408 (Hartree/Particle)
Thermal correction to Energy= 0.291307
Thermal correction to Enthalpy= 0.292251
Thermal correction to Gibbs Free Energy= 0.228807
Sum of electronic and zero-point Energies= -860.747097
Sum of electronic and thermal Energies= -860.730198
Sum of electronic and thermal Enthalpies= -860.729254
Sum of electronic and thermal Free Energies= -860.792698
SCF Done: E(RB3LYP) = -861.276209196 A.U. after 15 cycles

TS2 PhCCTS6pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.260992	1.176671	1.368754
2	6	0	-0.073553	0.835594	0.356954

3	6	0	-1.176486	0.286921	-0.417031
4	1	0	-1.007745	0.478184	-1.483125
5	6	0	1.019249	1.491511	-0.356396
6	6	0	-2.570517	0.834257	-0.027564
7	8	0	-2.829956	2.018304	0.131285
8	7	0	-3.468242	-0.188112	0.065430
9	6	0	-2.939384	-1.521762	-0.151054
10	1	0	-3.195985	-2.187304	0.684306
11	6	0	-1.450475	-1.320145	-0.268312
12	6	0	-0.423657	-2.102481	-0.225858
13	6	0	0.913954	-1.894434	0.028480
14	1	0	-3.358954	-1.966227	-1.066898
15	8	0	1.246295	1.401043	-1.555214
16	8	0	1.785157	2.239216	0.483018
17	6	0	2.879342	2.928074	-0.137151
18	1	0	3.392094	3.451866	0.670752
19	1	0	2.515104	3.642805	-0.880581
20	1	0	3.555865	2.221840	-0.625418
21	6	0	-4.877087	0.029350	0.322464
22	1	0	-5.486267	-0.321674	-0.520128
23	1	0	-5.031344	1.100340	0.459667
24	1	0	-5.192601	-0.504318	1.227515
25	6	0	1.201941	-1.047791	1.160935
26	6	0	2.548937	-0.683570	1.430388
27	6	0	3.549319	-1.059080	0.564445
28	6	0	3.262235	-1.857124	-0.581577
29	6	0	1.983180	-2.278182	-0.840521
30	1	0	0.470140	-0.979751	1.954322
31	1	0	2.777552	-0.114346	2.326124
32	1	0	4.578875	-0.776574	0.766970
33	1	0	4.071400	-2.134434	-1.251187
34	1	0	1.756584	-2.885642	-1.711007

SCF Done: E(RB3LYP) = -860.942136252 A.U. after 1 cycles
Zero-point correction= 0.271239 (Hartree/Particle)
Thermal correction to Energy= 0.288370
Thermal correction to Enthalpy= 0.289314
Thermal correction to Gibbs Free Energy= 0.225753
Sum of electronic and zero-point Energies= -860.670897
Sum of electronic and thermal Energies= -860.653767
Sum of electronic and thermal Enthalpies= -860.652822
Sum of electronic and thermal Free Energies= -860.716384
SCF Done: E(RB3LYP) = -861.201013082 A.U. after 16 cycles

M2 PhCCTS6pcm.rev.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.133723	1.183354	1.201231
2	6	0	0.141053	0.549348	0.354823
3	6	0	-1.132415	0.257587	-0.489677
4	1	0	-0.992782	0.694014	-1.486014
5	6	0	1.166529	1.308680	-0.471687
6	6	0	-2.418159	0.860438	0.101812
7	8	0	-2.544832	2.004215	0.522804
8	7	0	-3.401788	-0.087023	0.056308
9	6	0	-2.975431	-1.399163	-0.419189
10	1	0	-3.242739	-2.188471	0.297076
11	6	0	-1.482776	-1.231078	-0.566444
12	6	0	-0.476340	-2.081344	-0.523906
13	6	0	0.785760	-1.849033	-0.104418
14	1	0	-3.465672	-1.643559	-1.374932
15	8	0	1.370318	1.148131	-1.657950
16	8	0	1.843006	2.193177	0.287276
17	6	0	2.884263	2.923094	-0.386648
18	1	0	3.296617	3.600541	0.361102
19	1	0	2.472993	3.484194	-1.229102
20	1	0	3.654076	2.238036	-0.751031
21	6	0	-4.769101	0.175228	0.452778
22	1	0	-5.456921	0.010275	-0.386161
23	1	0	-4.831754	1.216177	0.773733
24	1	0	-5.067912	-0.478922	1.281568
25	6	0	0.821583	-0.779546	0.989855

26	6	0	2.186991	-0.543082	1.564203
27	6	0	3.291018	-1.081491	1.006542
28	6	0	3.210492	-1.952877	-0.152619
29	6	0	2.011955	-2.332296	-0.672841
30	1	0	0.142241	-1.049520	1.805319
31	1	0	2.258874	0.058402	2.466814
32	1	0	4.268537	-0.896243	1.444703
33	1	0	4.134271	-2.320534	-0.590849
34	1	0	1.955931	-3.009559	-1.520157

SCF Done: E(RB3LYP) = -860.963197763 A.U. after 1 cycles
Zero-point correction= 0.274055 (Hartree/Particle)
Thermal correction to Energy= 0.291056
Thermal correction to Enthalpy= 0.292000
Thermal correction to Gibbs Free Energy= 0.228721
Sum of electronic and zero-point Energies= -860.689143
Sum of electronic and thermal Energies= -860.672142
Sum of electronic and thermal Enthalpies= -860.671197
Sum of electronic and thermal Free Energies= -860.734476
SCF Done: E(RB3LYP) = -861.219516401 A.U. after 16 cycles

Scheme 13
3M1+H++H2O PhCCHwTS3pcm.rev.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.488090	-1.318989	-0.233171
2	6	0	-1.598186	-1.495489	0.932795
3	6	0	-0.191531	-1.228484	0.627940
4	6	0	-1.312529	0.756967	-0.878678
5	6	0	-2.379880	-0.282216	-1.084305
6	6	0	0.994897	-1.063878	0.423084
7	6	0	-1.506723	1.853199	-0.103582
8	8	0	-3.093978	-0.079330	-2.071894
9	6	0	-3.585717	-2.274412	-0.393666
10	1	0	-4.345522	-2.115866	0.380654
11	1	0	-3.196627	-3.291201	-0.306504
12	1	0	-4.035441	-2.122561	-1.374039
13	6	0	-0.570702	2.935044	-0.120508
14	6	0	2.384747	-0.852600	0.169757
15	6	0	3.113252	0.084071	0.930327
16	6	0	4.468985	0.284612	0.682045
17	6	0	5.114872	-0.439060	-0.324782
18	6	0	4.399378	-1.369095	-1.084707
19	6	0	3.043989	-1.579350	-0.841933
20	8	0	-0.666675	4.022959	0.568723
21	8	0	0.486757	2.847756	-0.877833
22	6	0	-1.792559	4.288295	1.464504
23	1	0	-1.806444	3.539761	2.256667
24	1	0	-2.718765	4.294036	0.889906
25	1	0	-1.582935	5.274811	1.869482
26	1	0	-0.461456	0.700189	-1.550129
27	1	0	-2.368668	1.940600	0.545288
28	1	0	-1.706321	-2.540868	1.247544
29	1	0	-1.935036	-0.864620	1.766279
30	1	0	2.608105	0.644930	1.710572
31	1	0	5.022676	1.007394	1.274337
32	1	0	6.172055	-0.279082	-0.516189
33	1	0	4.898759	-1.932871	-1.867363
34	1	0	2.485639	-2.302141	-1.428672
35	1	0	1.040641	3.652378	-0.803088
36	8	0	-1.863481	-4.820431	1.322494
37	1	0	-0.903458	-4.955018	1.367337
38	1	0	-2.145318	-4.890205	2.248452

SCF Done: E(RB3LYP) = -937.821674796 A.U. after 1 cycles
Zero-point correction= 0.306411 (Hartree/Particle)
Thermal correction to Energy= 0.330104
Thermal correction to Enthalpy= 0.331048
Thermal correction to Gibbs Free Energy= 0.248189
Sum of electronic and zero-point Energies= -937.515264
Sum of electronic and thermal Energies= -937.491571

```
 Sum of electronic and thermal Enthalpies=            -937.490627
 Sum of electronic and thermal Free Energies=         -937.573486
SCF Done:  E(RB3LYP) =  -938.118821628     A.U. after   17 cycles
```

TS3 PhCCHwTS3pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.937241	-0.561111	0.072412
2	6	0	-1.955439	-1.162067	0.970636
3	6	0	-0.596247	-0.862499	0.463952
4	6	0	-1.070174	0.794530	-0.694130
5	6	0	-2.531362	0.375748	-0.803529
6	6	0	0.609551	-1.114643	0.359614
7	6	0	-0.785443	1.988259	-0.020469
8	8	0	-3.224093	0.934738	-1.652463
9	6	0	-4.323487	-1.001808	0.146474
10	1	0	-4.759994	-0.722542	1.112326
11	1	0	-4.370680	-2.088595	0.033222
12	1	0	-4.877544	-0.514524	-0.655912
13	6	0	0.393758	2.690924	-0.264405
14	6	0	1.996191	-1.269632	0.172288
15	6	0	2.906413	-0.640716	1.055467
16	6	0	4.273527	-0.803567	0.870354
17	6	0	4.749615	-1.586317	-0.188284
18	6	0	3.857641	-2.213570	-1.066307
19	6	0	2.487671	-2.063509	-0.891426
20	8	0	0.747322	3.830965	0.278387
21	8	0	1.282922	2.211472	-1.115591
22	6	0	-0.128959	4.506924	1.217140
23	1	0	-0.284080	3.879902	2.097043
24	1	0	-1.076129	4.747673	0.731074
25	1	0	0.403561	5.416103	1.487115
26	1	0	-0.468348	0.545384	-1.562115
27	1	0	-1.471621	2.369277	0.724244
28	1	0	-2.117348	-2.247284	0.991007
29	1	0	-2.075192	-0.773379	1.991535
30	1	0	2.524229	-0.037038	1.872000
31	1	0	4.971797	-0.321923	1.547672
32	1	0	5.819478	-1.709162	-0.328569
33	1	0	4.234714	-2.819617	-1.884095
34	1	0	1.785691	-2.546521	-1.563107
35	1	0	2.038424	2.826068	-1.192584
36	8	0	-3.026795	-4.299422	0.552617
37	1	0	-2.231148	-4.693265	0.160612
38	1	0	-3.019512	-4.633148	1.463785

```
SCF Done:  E(RB3LYP) =  -937.816612331     A.U. after    1 cycles
Zero-point correction=                           0.305674 (Hartree/Particle)
 Thermal correction to Energy=                    0.328555
 Thermal correction to Enthalpy=                  0.329500
 Thermal correction to Gibbs Free Energy=         0.249165
 Sum of electronic and zero-point Energies=           -937.510938
 Sum of electronic and thermal Energies=              -937.488057
 Sum of electronic and thermal Enthalpies=            -937.487113
 Sum of electronic and thermal Free Energies=         -937.567447
SCF Done:  E(RB3LYP) =  -938.111554393     A.U. after   16 cycles
```

BM1+H++H2O PhCCHwTS3pcm.for.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.383038	-1.657389	0.149873
2	6	0	-1.139240	-1.741118	0.898491
3	6	0	-0.259958	-0.704827	0.212910
4	6	0	-1.216964	0.272535	-0.598613
5	6	0	-2.482043	-0.616135	-0.710001

6	6	0	1.010788	-0.606972	0.163691
7	6	0	-1.505267	1.546399	0.098887
8	8	0	-3.421603	-0.360904	-1.452575
9	6	0	-3.424313	-2.655706	0.325878
10	1	0	-3.847146	-2.597390	1.335624
11	1	0	-3.009291	-3.655804	0.169465
12	1	0	-4.207457	-2.454307	-0.406423
13	6	0	-0.982358	2.725443	-0.325061
14	6	0	2.366061	-0.401505	0.087526
15	6	0	3.012565	0.445871	1.040535
16	6	0	4.377582	0.647901	0.957342
17	6	0	5.113858	0.020879	-0.060583
18	6	0	4.495905	-0.815144	-1.004974
19	6	0	3.132803	-1.034060	-0.939816
20	8	0	-1.185176	3.938410	0.203043
21	8	0	-0.156029	2.781817	-1.384329
22	6	0	-2.066615	4.065298	1.330942
23	1	0	-1.677691	3.502559	2.184600
24	1	0	-3.069832	3.714718	1.071803
25	1	0	-2.088802	5.129086	1.563326
26	1	0	-0.800980	0.445322	-1.591441
27	1	0	-2.131829	1.526456	0.980525
28	1	0	-0.718350	-2.749839	0.834501
29	1	0	-1.285288	-1.478324	1.955314
30	1	0	2.418166	0.917033	1.815458
31	1	0	4.879803	1.288662	1.673937
32	1	0	6.185619	0.185191	-0.118649
33	1	0	5.088566	-1.287066	-1.781087
34	1	0	2.629621	-1.675673	-1.654737
35	1	0	0.061894	3.715081	-1.559141
36	8	0	-0.733873	-5.037276	0.431756
37	1	0	0.082851	-5.090328	-0.089585
38	1	0	-0.451984	-5.303184	1.321316

SCF Done: E(RB3LYP) = -937.826490416 A.U. after 1 cycles
Zero-point correction= 0.306852 (Hartree/Particle)
Thermal correction to Energy= 0.329827
Thermal correction to Enthalpy= 0.330771
Thermal correction to Gibbs Free Energy= 0.250478
Sum of electronic and zero-point Energies= -937.519639
Sum of electronic and thermal Energies= -937.496664
Sum of electronic and thermal Enthalpies= -937.495719
Sum of electronic and thermal Free Energies= -937.576012
SCF Done: E(RB3LYP) = -938.121627182 A.U. after 16 cycles

CM1+H+ PhCCHw1pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.344142	-0.570236	0.008287
2	6	0	2.452560	-1.695076	-0.215302
3	6	0	1.073561	-1.098117	-0.012307
4	6	0	1.205895	0.359719	0.412951
5	6	0	2.731514	0.597903	0.341333
6	6	0	-0.080307	-1.728147	-0.184496
7	6	0	0.409864	1.351226	-0.386906
8	8	0	3.290154	1.665852	0.564017
9	6	0	4.781331	-0.716417	-0.112811
10	1	0	5.053346	-1.037310	-1.125147
11	1	0	5.157872	-1.455926	0.603584
12	1	0	5.234456	0.253731	0.095189
13	6	0	-0.426377	2.232065	0.191477
14	6	0	-1.488711	-1.383775	0.028699
15	6	0	-2.398778	-1.367354	-1.044246
16	6	0	-3.734952	-1.045983	-0.819723
17	6	0	-4.172854	-0.732814	0.470936
18	6	0	-3.274249	-0.746001	1.539908
19	6	0	-1.937109	-1.077330	1.324568
20	8	0	-1.197172	3.156733	-0.421263
21	8	0	-0.593353	2.292174	1.534949
22	6	0	-1.211950	3.180771	-1.852175
23	1	0	-1.539091	2.214206	-2.249319

24	1	0	-0.220230	3.427459	-2.245465
25	1	0	-1.923561	3.958852	-2.127850
26	1	0	0.932814	0.454347	1.471004
27	1	0	0.542972	1.360764	-1.460699
28	1	0	2.647785	-2.507704	0.498314
29	1	0	2.585123	-2.106195	-1.224821
30	1	0	-2.058736	-1.589798	-2.051781
31	1	0	-4.432425	-1.031468	-1.651608
32	1	0	-5.214895	-0.478866	0.641863
33	1	0	-3.614603	-0.507285	2.542891
34	1	0	-1.239268	-1.104591	2.155210
35	1	0	-1.332654	2.897383	1.718624
36	8	0	0.117981	-3.170417	-0.669375
37	1	0	-0.447759	-3.807325	-0.175900
38	1	0	-0.057635	-3.287365	-1.630159

SCF Done: E(RB3LYP) = -937.838474774 A.U. after 1 cycles
Zero-point correction= 0.311799 (Hartree/Particle)
Thermal correction to Energy= 0.332160
Thermal correction to Enthalpy= 0.333104
Thermal correction to Gibbs Free Energy= 0.261272
Sum of electronic and zero-point Energies= -937.526675
Sum of electronic and thermal Energies= -937.506315
Sum of electronic and thermal Enthalpies= -937.505371
Sum of electronic and thermal Free Energies= -937.577203
SCF Done: E(RB3LYP) = -938.126500910 A.U. after 15 cycles

5Mt+H+ PhCCHwtpcm.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.964073	-1.516855	-0.186832
2	6	0	1.614913	-2.015216	0.018555
3	6	0	0.739719	-0.727467	-0.122337
4	6	0	1.713724	0.417932	0.268815
5	6	0	3.095767	-0.172715	-0.041396
6	6	0	-0.494734	-0.793777	0.717530
7	6	0	1.486320	1.747413	-0.444877
8	8	0	4.135477	0.473242	-0.120818
9	6	0	4.087606	-2.419808	-0.355991
10	1	0	3.939366	-3.052653	-1.237338
11	1	0	4.208187	-3.061768	0.524737
12	1	0	4.985627	-1.814549	-0.487997
13	6	0	0.163226	2.382438	-0.080689
14	6	0	-1.829403	-0.998790	0.214895
15	6	0	-2.035345	-1.430007	-1.116840
16	6	0	-3.321822	-1.672180	-1.580132
17	6	0	-4.418780	-1.465570	-0.738920
18	6	0	-4.232428	-1.020282	0.576657
19	6	0	-2.952363	-0.793780	1.054525
20	8	0	0.089163	3.649799	-0.489348
21	8	0	-0.741909	1.805127	0.504004
22	6	0	-1.153591	4.340876	-0.226284
23	1	0	-1.333604	4.395119	0.849403
24	1	0	-1.983015	3.824450	-0.713926
25	1	0	-1.021850	5.337658	-0.644307
26	1	0	1.678452	0.579949	1.352691
27	1	0	1.514036	1.618908	-1.534953
28	1	0	1.510119	-2.476527	1.008839
29	1	0	1.352460	-2.759561	-0.738542
30	1	0	-1.196397	-1.606981	-1.778625
31	1	0	-3.470282	-2.018729	-2.597084
32	1	0	-5.423623	-1.644839	-1.108525
33	1	0	-5.087588	-0.844184	1.220029
34	1	0	-2.840839	-0.408732	2.064192
35	1	0	2.299578	2.437119	-0.199136
36	8	0	-0.243253	-0.761226	1.991714
37	1	0	-1.033903	-0.892605	2.551826
38	1	0	0.462078	-0.604033	-1.168941

SCF Done: E(RB3LYP) = -937.939109500 A.U. after 1 cycles
Zero-point correction= 0.315284 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.334552
 Thermal correction to Enthalpy=                0.335496
 Thermal correction to Gibbs Free Energy=       0.265980
 Sum of electronic and zero-point Energies=           -937.623825
 Sum of electronic and thermal Energies=              -937.604557
 Sum of electronic and thermal Enthalpies=            -937.603613
 Sum of electronic and thermal Free Energies=         -937.673130
SCF Done:  E(RB3LYP) =  -938.211682078     A.U. after   16 cycles
```

```
5Mc+H+         PhCCHwcpcm.log
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -2.895261   -1.370665   -0.349024
      2          6           0       -1.726646   -1.725899   -1.133511
      3          6           0       -0.693415   -0.590316   -0.813946
      4          6           0       -1.621656    0.597754   -0.412408
      5          6           0       -2.905694   -0.082444    0.083563
      6          6           0        0.228293   -1.065133    0.262297
      7          6           0       -1.108936    1.666569    0.549633
      8          8           0       -3.793898    0.465112    0.728257
      9          6           0       -4.007079   -2.286875   -0.177006
     10          1           0       -3.672528   -3.204835    0.318152
     11          1           0       -4.451451   -2.548071   -1.144565
     12          1           0       -4.755849   -1.790848    0.442257
     13          6           0       -0.027549    2.536675   -0.058524
     14          6           0        1.645517   -1.225417    0.115471
     15          6           0        2.347504   -0.488394   -0.872656
     16          6           0        3.724333   -0.619134   -0.983151
     17          6           0        4.414960   -1.498882   -0.143398
     18          6           0        3.732383   -2.246409    0.826964
     19          6           0        2.362815   -2.106583    0.968172
     20          8           0        0.239561    3.592154    0.720236
     21          8           0        0.539129    2.309716   -1.113523
     22          6           0        1.278331    4.481113    0.254802
     23          1           0        1.003019    4.911851   -0.710353
     24          1           0        2.223434    3.941860    0.159740
     25          1           0        1.354729    5.258640    1.013624
     26          1           0       -1.885421    1.094651   -1.354966
     27          1           0       -0.728363    1.238287    1.484516
     28          1           0       -1.940823   -1.719119   -2.209626
     29          1           0       -1.367192   -2.724580   -0.866691
     30          1           0        1.826353    0.227671   -1.495994
     31          1           0        4.261973   -0.036268   -1.723034
     32          1           0        5.490298   -1.607406   -0.244833
     33          1           0        4.272656   -2.939866    1.461930
     34          1           0        1.850722   -2.730416    1.695262
     35          1           0       -1.954424    2.297922    0.842326
     36          8           0       -0.387110   -1.383294    1.364579
     37          1           0        0.214242   -1.668563    2.082848
     38          1           0       -0.114969   -0.355515   -1.701625
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -937.933475662     A.U. after    1 cycles
Zero-point correction=                           0.315059 (Hartree/Particle)
 Thermal correction to Energy=                    0.334416
 Thermal correction to Enthalpy=                  0.335361
 Thermal correction to Gibbs Free Energy=         0.264686
 Sum of electronic and zero-point Energies=           -937.618416
 Sum of electronic and thermal Energies=              -937.599059
 Sum of electronic and thermal Enthalpies=            -937.598115
 Sum of electronic and thermal Free Energies=         -937.668790
SCF Done:  E(RB3LYP) =  -938.206022014     A.U. after   18 cycles
```

```
Scheme 14
6M1+H2O     diEPhCCwTS1pcm.for3.log
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
```

1	6	0	3.692555	-0.117385	0.638602
2	6	0	2.470117	0.525500	0.033900
3	6	0	1.324470	-0.125510	-0.218144
4	1	0	0.492599	0.458686	-0.597312
5	6	0	2.527644	1.996154	-0.251594
6	6	0	1.151186	-1.581980	0.073174
7	8	0	1.914206	-2.156564	0.858804
8	7	0	0.107718	-2.217091	-0.535391
9	6	0	-0.728366	-1.602702	-1.578305
10	1	0	-1.062762	-2.410910	-2.237826
11	1	0	-0.119487	-0.943298	-2.203752
12	6	0	-1.889107	-0.864453	-1.059052
13	6	0	-2.830294	-0.218155	-0.642513
14	6	0	-3.927658	0.570043	-0.166900
15	8	0	1.581117	2.660702	-0.627927
16	8	0	4.033217	0.058766	1.789513
17	8	0	4.373609	-0.829752	-0.266210
18	6	0	5.555100	-1.497860	0.225601
19	1	0	5.990190	-1.992781	-0.641669
20	1	0	5.278775	-2.230307	0.987681
21	1	0	6.254908	-0.773174	0.647446
22	8	0	3.762809	2.480871	-0.059358
23	6	0	3.939055	3.889686	-0.320446
24	1	0	4.988511	4.092569	-0.112578
25	1	0	3.294471	4.477276	0.336854
26	1	0	3.701448	4.111509	-1.363151
27	6	0	-0.189311	-3.608623	-0.196467
28	1	0	-1.259826	-3.719200	0.004082
29	1	0	0.380429	-3.879307	0.690567
30	1	0	0.090628	-4.274294	-1.021849
31	6	0	-3.913224	1.968766	-0.335706
32	6	0	-4.979916	2.739759	0.120682
33	6	0	-6.069567	2.131243	0.750237
34	6	0	-6.089635	0.744386	0.922552
35	6	0	-5.029236	-0.036914	0.468131
36	1	0	-3.064713	2.438160	-0.823822
37	1	0	-4.960071	3.817374	-0.014344
38	1	0	-6.899154	2.735729	1.105762
39	1	0	-6.934342	0.268622	1.412579
40	1	0	-5.039361	-1.114286	0.603678
41	8	0	-3.730109	-3.312785	0.377412
42	1	0	-3.306941	-2.511962	0.021188
43	1	0	-4.140983	-3.712389	-0.406183

SCF Done: E(RB3LYP) = -1165.29495720 A.U. after 1 cycles
Zero-point correction= 0.338215 (Hartree/Particle)
Thermal correction to Energy= 0.365377
Thermal correction to Enthalpy= 0.366322
Thermal correction to Gibbs Free Energy= 0.275589
Sum of electronic and zero-point Energies= -1164.956742
Sum of electronic and thermal Energies= -1164.929580
Sum of electronic and thermal Enthalpies= -1164.928636
Sum of electronic and thermal Free Energies= -1165.019368
SCF Done: E(RB3LYP) = -1165.66294833 A.U. after 15 cycles

TS4 diEPhCCwTS1pcm.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.109081	1.562231	0.671522
2	6	0	-1.134523	1.260636	-0.374839
3	6	0	-0.990588	-0.039403	-0.932115
4	1	0	-0.379548	-0.019301	-1.832290
5	6	0	-0.144896	2.231619	-0.844738
6	6	0	-2.219421	-0.936274	-1.124706
7	8	0	-3.118570	-0.609690	-1.895343
8	7	0	-2.149540	-2.097013	-0.437354
9	6	0	-1.042620	-2.241528	0.490454
10	1	0	-0.608537	-3.245562	0.422943
11	1	0	-1.373406	-2.062968	1.523192
12	6	0	-0.012695	-1.225588	0.094508
13	6	0	1.219645	-1.033638	0.198388

14	6	0	2.561467	-0.646139	0.281622
15	8	0	0.745789	1.949080	-1.647419
16	8	0	-2.466517	2.662099	1.069825
17	8	0	-2.632671	0.413415	1.202157
18	6	0	-3.664313	0.594072	2.183133
19	1	0	-3.974056	-0.410942	2.470844
20	1	0	-4.509193	1.145534	1.761810
21	1	0	-3.281303	1.135816	3.052099
22	8	0	-0.255222	3.473120	-0.319547
23	6	0	0.732747	4.417684	-0.759228
24	1	0	0.485643	5.351781	-0.253716
25	1	0	0.690355	4.550412	-1.843638
26	1	0	1.737596	4.089357	-0.479192
27	6	0	-3.231766	-3.063224	-0.430436
28	1	0	-2.847371	-4.066414	-0.642864
29	1	0	-3.947081	-2.774614	-1.201353
30	1	0	-3.735244	-3.077510	0.544417
31	6	0	2.989164	0.215866	1.324892
32	6	0	4.324313	0.585847	1.414461
33	6	0	5.249266	0.109912	0.476760
34	6	0	4.840416	-0.743296	-0.556506
35	6	0	3.510220	-1.125817	-0.658086
36	1	0	2.261883	0.576635	2.044648
37	1	0	4.650011	1.245781	2.212526
38	1	0	6.292198	0.403154	0.552137
39	1	0	5.564550	-1.107987	-1.278346
40	1	0	3.181244	-1.787591	-1.452671
41	8	0	1.048459	-4.868702	0.130052
42	1	0	1.487251	-4.316283	-0.536269
43	1	0	1.517632	-4.642535	0.948889

```
SCF Done:  E(RB3LYP) =  -1165.26667678     A.U. after    1 cycles
Zero-point correction=                           0.335747 (Hartree/Particle)
 Thermal correction to Energy=                    0.362685
 Thermal correction to Enthalpy=                  0.363630
 Thermal correction to Gibbs Free Energy=         0.274234
 Sum of electronic and zero-point Energies=          -1164.930929
 Sum of electronic and thermal Energies=             -1164.903991
 Sum of electronic and thermal Enthalpies=           -1164.903047
 Sum of electronic and thermal Free Energies=        -1164.992442
SCF Done:  E(RB3LYP) =  -1165.63589612     A.U. after   16 cycles
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BM2+H2O diEPhCCwTS2pcm.for.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.203881	1.378175	0.746428
2	6	0	-1.263262	1.203224	-0.342892
3	6	0	-0.962244	-0.103286	-0.913282
4	1	0	-0.437661	0.036549	-1.858995
5	6	0	-0.410116	2.268060	-0.836729
6	6	0	-2.134988	-1.080594	-1.131826
7	8	0	-3.080620	-0.827424	-1.870703
8	7	0	-1.931200	-2.242208	-0.466167
9	6	0	-0.787109	-2.259904	0.424912
10	1	0	-0.219449	-3.191433	0.325923
11	1	0	-1.098332	-2.133288	1.471056
12	6	0	0.051406	-1.075886	-0.018347
13	6	0	1.286837	-0.822974	0.103836
14	6	0	2.607270	-0.422873	0.237440
15	8	0	0.523603	2.073736	-1.624031
16	8	0	-2.619619	2.424313	1.233368
17	8	0	-2.630002	0.163166	1.234294
18	6	0	-3.613971	0.223001	2.273825
19	1	0	-3.849309	-0.814071	2.516392
20	1	0	-4.512851	0.744160	1.932359
21	1	0	-3.219933	0.736272	3.155561
22	8	0	-0.684018	3.513303	-0.369817
23	6	0	0.188751	4.549867	-0.838641
24	1	0	-0.174531	5.467647	-0.374135
25	1	0	0.147124	4.636511	-1.928137
26	1	0	1.222971	4.358810	-0.537828

27	6	0	-2.905642	-3.315055	-0.437760
28	1	0	-2.427052	-4.272257	-0.670226
29	1	0	-3.668067	-3.095966	-1.186640
30	1	0	-3.378406	-3.387750	0.549879
31	6	0	2.996907	0.396752	1.335267
32	6	0	4.321755	0.779005	1.474540
33	6	0	5.274387	0.362213	0.534298
34	6	0	4.906646	-0.444965	-0.552171
35	6	0	3.588526	-0.842832	-0.705418
36	1	0	2.245646	0.710329	2.052128
37	1	0	4.621113	1.402850	2.310642
38	1	0	6.310369	0.666684	0.649369
39	1	0	5.655516	-0.760334	-1.271545
40	1	0	3.286752	-1.469498	-1.538024
41	8	0	1.439144	-4.819392	0.037827
42	1	0	1.975555	-4.225092	-0.510652
43	1	0	1.803404	-4.687862	0.927654

SCF Done: E(RB3LYP) = -1165.26746346 A.U. after 1 cycles
Zero-point correction= 0.336715 (Hartree/Particle)
Thermal correction to Energy= 0.363828
Thermal correction to Enthalpy= 0.364773
Thermal correction to Gibbs Free Energy= 0.275059
Sum of electronic and zero-point Energies= -1164.930748
Sum of electronic and thermal Energies= -1164.903635
Sum of electronic and thermal Enthalpies= -1164.902691
Sum of electronic and thermal Free Energies= -1164.992405
SCF Done: E(RB3LYP) = -1165.63707191 A.U. after 16 cycles

TS5 diEPhCCwTS2pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.957652	1.561085	1.133495
2	6	0	-0.453505	1.263031	-0.174440
3	6	0	-0.955913	0.077612	-0.927402
4	1	0	-0.482698	0.111807	-1.914278
5	6	0	0.555395	2.028028	-0.854619
6	6	0	-2.482934	0.026682	-1.159561
7	8	0	-3.134373	0.939199	-1.656411
8	7	0	-2.973239	-1.185374	-0.790288
9	6	0	-2.019548	-2.066902	-0.148250
10	1	0	-2.004301	-3.052942	-0.624798
11	1	0	-2.251754	-2.206236	0.915741
12	6	0	-0.698848	-1.352348	-0.316365
13	6	0	0.503934	-1.766526	-0.087799
14	6	0	1.884215	-1.506280	0.057144
15	8	0	1.011824	1.758361	-1.976928
16	8	0	-0.686342	2.489022	1.896903
17	8	0	-1.886252	0.599514	1.530943
18	6	0	-2.475166	0.807160	2.814660
19	1	0	-3.177761	-0.016425	2.956336
20	1	0	-3.007192	1.762674	2.859047
21	1	0	-1.719431	0.791928	3.606449
22	8	0	1.011665	3.131511	-0.181214
23	6	0	2.009222	3.893288	-0.865262
24	1	0	2.261112	4.715833	-0.192765
25	1	0	1.630262	4.289907	-1.812514
26	1	0	2.901039	3.292856	-1.070328
27	6	0	-4.379432	-1.527016	-0.852762
28	1	0	-4.526994	-2.459174	-1.409993
29	1	0	-4.898208	-0.712936	-1.361075
30	1	0	-4.797231	-1.650492	0.154407
31	6	0	2.325186	-0.731070	1.157728
32	6	0	3.673188	-0.411635	1.280430
33	6	0	4.587678	-0.871030	0.327344
34	6	0	4.163234	-1.647556	-0.760347
35	6	0	2.820512	-1.966661	-0.900699
36	1	0	1.601312	-0.388284	1.888576
37	1	0	4.013712	0.190187	2.116958
38	1	0	5.640159	-0.623527	0.430350
39	1	0	4.883656	-1.994379	-1.494194
40	1	0	2.475018	-2.560289	-1.740896

41	8	0	0.216520	-3.672365	0.687458
42	1	0	0.592891	-4.281684	0.026555
43	1	0	0.817363	-3.732301	1.452678

SCF Done: E(RB3LYP) = -1165.26320681 A.U. after 1 cycles
Zero-point correction= 0.338770 (Hartree/Particle)
Thermal correction to Energy= 0.363631
Thermal correction to Enthalpy= 0.364575
Thermal correction to Gibbs Free Energy= 0.282440
Sum of electronic and zero-point Energies= -1164.924436
Sum of electronic and thermal Energies= -1164.899576
Sum of electronic and thermal Enthalpies= -1164.898632
Sum of electronic and thermal Free Energies= -1164.980767
SCF Done: E(RB3LYP) = -1165.62928936 A.U. after 18 cycles

CM2 diEPhCCwTS2pcm.rev.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.720195	1.506509	1.202785
2	6	0	-0.281647	1.202618	-0.119163
3	6	0	-0.923118	0.069052	-0.885468
4	1	0	-0.412566	0.047594	-1.857118
5	6	0	0.741312	1.907662	-0.825757
6	6	0	-2.424174	0.247438	-1.181968
7	8	0	-2.940965	1.247053	-1.673306
8	7	0	-3.085551	-0.898518	-0.854705
9	6	0	-2.270351	-1.903359	-0.199233
10	1	0	-2.346534	-2.871370	-0.710734
11	1	0	-2.583616	-2.050898	0.843777
12	6	0	-0.871366	-1.326778	-0.274559
13	6	0	0.237232	-1.949305	0.093063
14	6	0	1.670827	-1.636900	0.106070
15	8	0	1.126197	1.647439	-1.979751
16	8	0	-0.339588	2.371360	1.997198
17	8	0	-1.746690	0.634984	1.593114
18	6	0	-2.268816	0.852327	2.901670
19	1	0	-3.053939	0.105402	3.038490
20	1	0	-2.691782	1.857212	3.002545
21	1	0	-1.497280	0.723408	3.668116
22	8	0	1.320683	2.951435	-0.140306
23	6	0	2.339646	3.654091	-0.851486
24	1	0	2.682279	4.439191	-0.173606
25	1	0	1.952901	4.102622	-1.772394
26	1	0	3.176515	2.997282	-1.110638
27	6	0	-4.519220	-1.058746	-0.971530
28	1	0	-4.764101	-1.956747	-1.550805
29	1	0	-4.913407	-0.178704	-1.481936
30	1	0	-4.987445	-1.143134	0.017796
31	6	0	2.242820	-0.966705	1.201943
32	6	0	3.610018	-0.696314	1.217979
33	6	0	4.415004	-1.093808	0.146473
34	6	0	3.854091	-1.760429	-0.945841
35	6	0	2.486713	-2.032495	-0.968510
36	1	0	1.611176	-0.650795	2.025966
37	1	0	4.046611	-0.173229	2.063493
38	1	0	5.479984	-0.880192	0.161428
39	1	0	4.478822	-2.063623	-1.780624
40	1	0	2.044911	-2.542174	-1.819844
41	8	0	-0.064159	-3.360114	0.672278
42	1	0	0.404862	-4.066112	0.173888
43	1	0	0.214992	-3.432490	1.612527

SCF Done: E(RB3LYP) = -1165.26985428 A.U. after 1 cycles
Zero-point correction= 0.341559 (Hartree/Particle)
Thermal correction to Energy= 0.366096
Thermal correction to Enthalpy= 0.367040
Thermal correction to Gibbs Free Energy= 0.285713
Sum of electronic and zero-point Energies= -1164.928295
Sum of electronic and thermal Energies= -1164.903758
Sum of electronic and thermal Enthalpies= -1164.902814
Sum of electronic and thermal Free Energies= -1164.984141

SCF Done: E(RB3LYP) = -1165.63493466   A.U. after   16 cycles

7Mc diEPhCCwp1pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.923013	0.549906	1.451005
2	6	0	-0.527279	0.916868	0.022049
3	6	0	-0.426859	-0.226985	-1.024300
4	1	0	-0.134913	0.276029	-1.950405
5	6	0	-1.418089	2.030961	-0.552176
6	6	0	-1.778088	-0.912334	-1.280381
7	8	0	-2.794002	-0.332286	-1.661660
8	7	0	-1.649832	-2.238316	-1.036274
9	6	0	-0.380920	-2.612906	-0.425761
10	1	0	-0.002189	-3.540382	-0.867663
11	1	0	-0.496015	-2.764112	0.652858
12	6	0	0.546048	-1.417421	-0.733556
13	6	0	1.585738	-1.162544	0.359529
14	6	0	2.822738	-0.393768	0.025441
15	8	0	-1.184146	2.578227	-1.609013
16	8	0	-0.465538	1.108296	2.426846
17	8	0	-1.836612	-0.428158	1.503151
18	6	0	-2.270713	-0.817103	2.823981
19	1	0	-3.003354	-1.607356	2.666987
20	1	0	-2.724345	0.033829	3.336636
21	1	0	-1.421728	-1.187146	3.402711
22	8	0	-2.435351	2.344965	0.257296
23	6	0	-3.317827	3.388963	-0.209971
24	1	0	-4.060609	3.512729	0.576702
25	1	0	-3.792726	3.083907	-1.144847
26	1	0	-2.759575	4.314713	-0.363655
27	6	0	-2.767099	-3.160393	-1.081735
28	1	0	-2.502294	-4.052229	-1.659730
29	1	0	-3.608208	-2.653762	-1.557327
30	1	0	-3.057729	-3.471605	-0.070103
31	6	0	3.737916	-0.136407	1.062940
32	6	0	4.904941	0.578388	0.816494
33	6	0	5.175695	1.051041	-0.472557
34	6	0	4.274575	0.804903	-1.510482
35	6	0	3.104893	0.085506	-1.265628
36	1	0	3.511863	-0.507188	2.056932
37	1	0	5.604366	0.770101	1.625009
38	1	0	6.086897	1.609960	-0.666166
39	1	0	4.481644	1.170664	-2.511726
40	1	0	2.421822	-0.094713	-2.088744
41	8	0	1.392575	-1.567516	1.501719
42	1	0	0.462850	1.376892	0.107701
43	1	0	1.071701	-1.630384	-1.667324

SCF Done: E(RB3LYP) = -1165.39236964   A.U. after   1 cycles
Zero-point correction=   0.345586 (Hartree/Particle)
 Thermal correction to Energy=   0.369193
 Thermal correction to Enthalpy=   0.370138
 Thermal correction to Gibbs Free Energy=   0.289939
 Sum of electronic and zero-point Energies=   -1165.046784
 Sum of electronic and thermal Energies=   -1165.023176
 Sum of electronic and thermal Enthalpies=   -1165.022232
 Sum of electronic and thermal Free Energies=   -1165.102430
SCF Done: E(RB3LYP) = -1165.73904242   A.U. after   16 cycles

7Mt diEPhCCwp2pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.590230	-1.194887	-1.214672
2	6	0	-1.463823	-0.968427	0.289717
3	6	0	-0.684185	0.283223	0.737165

4	1	0	-0.609367	0.210655	1.829021
5	6	0	-2.824594	-1.007871	1.000928
6	6	0	-1.373060	1.616119	0.438849
7	8	0	-2.580313	1.836299	0.512455
8	7	0	-0.407886	2.524554	0.138598
9	6	0	0.947427	1.993885	0.199490
10	1	0	1.448543	2.317559	1.123245
11	1	0	1.541027	2.351732	-0.647204
12	6	0	0.732992	0.451500	0.167591
13	6	0	1.806985	-0.304328	0.954498
14	6	0	3.184625	-0.412098	0.387968
15	8	0	-2.938784	-0.932551	2.206143
16	8	0	-1.565401	-2.295257	-1.727723
17	8	0	-1.727468	-0.050950	-1.901134
18	6	0	-1.880390	-0.183665	-3.330551
19	1	0	-1.950097	0.834781	-3.710032
20	1	0	-2.790141	-0.742997	-3.559998
21	1	0	-1.016524	-0.696787	-3.758457
22	8	0	-3.844064	-1.186242	0.151801
23	6	0	-5.158925	-1.244993	0.745613
24	1	0	-5.844127	-1.411024	-0.084506
25	1	0	-5.383697	-0.301633	1.248113
26	1	0	-5.214405	-2.067111	1.462253
27	6	0	-0.663265	3.942940	-0.017850
28	1	0	-0.220324	4.514687	0.807269
29	1	0	-1.743960	4.092720	-0.020025
30	1	0	-0.242116	4.306356	-0.961729
31	6	0	4.188287	-0.978010	1.194861
32	6	0	5.490640	-1.100369	0.722495
33	6	0	5.810077	-0.662003	-0.567518
34	6	0	4.821812	-0.102086	-1.379784
35	6	0	3.515742	0.023766	-0.906226
36	1	0	3.924364	-1.313236	2.192271
37	1	0	6.258365	-1.536027	1.355392
38	1	0	6.826832	-0.758176	-0.937823
39	1	0	5.065746	0.235271	-2.382731
40	1	0	2.762507	0.454307	-1.557222
41	8	0	1.537495	-0.792185	2.046781
42	1	0	-0.924366	-1.843517	0.668603
43	1	0	0.754538	0.131478	-0.878653

```
SCF Done:  E(RB3LYP) =  -1165.39679424     A.U. after    1 cycles
Zero-point correction=                           0.345090 (Hartree/Particle)
 Thermal correction to Energy=                    0.368892
 Thermal correction to Enthalpy=                  0.369836
 Thermal correction to Gibbs Free Energy=         0.288758
 Sum of electronic and zero-point Energies=          -1165.051704
 Sum of electronic and thermal Energies=             -1165.027902
 Sum of electronic and thermal Enthalpies=           -1165.026958
 Sum of electronic and thermal Free Energies=        -1165.108036
SCF Done:  E(RB3LYP) =  -1165.74443350     A.U. after   14 cycles
```

Scheme 15

6M2+H++H2O diEHCCHwTS1pcm.for3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807035	-1.804872	-0.286546
2	6	0	0.186314	-0.906111	0.290732
3	6	0	-0.111150	0.324775	0.790712
4	1	0	0.700034	0.879082	1.249625
5	6	0	1.588798	-1.408799	0.281979
6	6	0	-1.479491	0.896821	1.048231
7	8	0	-1.961720	0.555360	2.131118
8	7	0	-2.029735	1.758946	0.171934
9	6	0	-1.426538	2.081054	-1.134569
10	1	0	-1.887151	3.015377	-1.470720
11	1	0	-1.695850	1.313396	-1.872771
12	6	0	0.026902	2.249715	-1.074843
13	6	0	1.227453	2.405025	-1.045322
14	1	0	2.301324	2.492667	-0.965136
15	8	0	1.875834	-2.546831	-0.114501

16	8	0	-0.498155	-2.981418	-0.693830
17	8	0	-2.026260	-1.400111	-0.378011
18	6	0	-3.043104	-2.296645	-0.938126
19	1	0	-3.964360	-1.723685	-0.880833
20	1	0	-3.094450	-3.199298	-0.330033
21	1	0	-2.779865	-2.529521	-1.969570
22	8	0	2.469661	-0.529203	0.695406
23	6	0	3.878295	-0.895740	0.674671
24	1	0	4.405866	0.055679	0.653128
25	1	0	4.092782	-1.487190	-0.215302
26	1	0	4.106255	-1.466332	1.576612
27	6	0	-3.369757	2.287134	0.427607
28	1	0	-3.346840	3.380997	0.411921
29	1	0	-3.696476	1.942305	1.407428
30	1	0	-4.068394	1.930281	-0.336784
31	8	0	4.286007	2.306579	-0.483698
32	1	0	4.812450	2.223368	-1.294798
33	1	0	4.611934	3.126695	-0.079397
34	1	0	0.523811	-3.095581	-0.545917

SCF Done: E(RB3LYP) = -934.641891758 A.U. after 1 cycles
Zero-point correction= 0.266762 (Hartree/Particle)
Thermal correction to Energy= 0.289544
Thermal correction to Enthalpy= 0.290488
Thermal correction to Gibbs Free Energy= 0.213240
Sum of electronic and zero-point Energies= -934.375129
Sum of electronic and thermal Energies= -934.352348
Sum of electronic and thermal Enthalpies= -934.351403
Sum of electronic and thermal Free Energies= -934.428652
SCF Done: E(RB3LYP) = -934.948717142 A.U. after 16 cycles

TS6 diEHCCHwTS1pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.569519	-1.643398	-0.686445
2	6	0	0.914516	-0.566295	0.181143
3	6	0	-0.038660	0.191785	0.895101
4	1	0	0.383402	0.834638	1.659558
5	6	0	2.338084	-0.221114	0.240594
6	6	0	-1.375402	-0.412745	1.330818
7	8	0	-1.344495	-1.261243	2.215917
8	7	0	-2.469605	0.079564	0.721594
9	6	0	-2.292102	1.055276	-0.343934
10	1	0	-3.037407	1.851814	-0.245405
11	1	0	-2.421811	0.588552	-1.329979
12	6	0	-0.934787	1.634357	-0.222987
13	6	0	-0.093608	2.521913	-0.378842
14	1	0	0.797791	3.110916	-0.391564
15	8	0	3.225028	-0.884899	-0.320780
16	8	0	1.458375	-2.362136	-1.297091
17	8	0	-0.687009	-1.925066	-0.881148
18	6	0	-1.036550	-3.047494	-1.745032
19	1	0	-2.122943	-3.079865	-1.721142
20	1	0	-0.605912	-3.964722	-1.342858
21	1	0	-0.669937	-2.856752	-2.753940
22	8	0	2.599233	0.878430	0.936710
23	6	0	3.990517	1.270214	1.045769
24	1	0	3.980235	2.181277	1.640823
25	1	0	4.402976	1.457385	0.053074
26	1	0	4.558927	0.484684	1.546490
27	6	0	-3.800975	-0.439562	0.997552
28	1	0	-4.469416	0.374528	1.294911
29	1	0	-3.720268	-1.162147	1.809536
30	1	0	-4.208993	-0.932455	0.108271
31	8	0	-0.824834	4.511236	-1.719946
32	1	0	-1.203306	4.050800	-2.486645
33	1	0	-1.604032	4.766918	-1.199635
34	1	0	2.374224	-1.970699	-1.044362

SCF Done: E(RB3LYP) = -934.626685424 A.U. after 1 cycles
Zero-point correction= 0.266771 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.288568
 Thermal correction to Enthalpy=                0.289512
 Thermal correction to Gibbs Free Energy=       0.214618
 Sum of electronic and zero-point Energies=          -934.359915
 Sum of electronic and thermal Energies=             -934.338117
 Sum of electronic and thermal Enthalpies=           -934.337173
 Sum of electronic and thermal Free Energies=        -934.412067
SCF Done:  E(RB3LYP) =  -934.931661475     A.U. after   16 cycles
```

CM3+H+ diEHCCHwTS1pcm.rev.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.801687	-1.503378	-0.320785
2	6	0	0.988318	-0.187351	0.078366
3	6	0	-0.189164	0.698181	0.385774
4	1	0	0.204871	1.646406	0.772922
5	6	0	2.349335	0.265274	0.203935
6	6	0	-1.144362	0.177404	1.484430
7	8	0	-0.798095	-0.337421	2.539350
8	7	0	-2.422361	0.441356	1.099252
9	6	0	-2.559832	1.029349	-0.222900
10	1	0	-2.969552	2.048764	-0.168014
11	1	0	-3.241096	0.433935	-0.845344
12	6	0	-1.141932	1.030831	-0.753229
13	6	0	-0.723452	1.265899	-1.983955
14	1	0	0.275263	1.254518	-2.389351
15	8	0	3.350505	-0.448664	-0.021782
16	8	0	1.780575	-2.341611	-0.586736
17	8	0	-0.433015	-1.965103	-0.456084
18	6	0	-0.618318	-3.341394	-0.861731
19	1	0	-1.697705	-3.480479	-0.890199
20	1	0	-0.164022	-4.016150	-0.133890
21	1	0	-0.184120	-3.506602	-1.849625
22	8	0	2.482794	1.546670	0.585668
23	6	0	3.828808	2.042795	0.721135
24	1	0	3.720902	3.082805	1.027232
25	1	0	4.357832	1.977171	-0.232259
26	1	0	4.370984	1.474842	1.480463
27	6	0	-3.583734	0.163631	1.921861
28	1	0	-4.130485	1.086850	2.145256
29	1	0	-3.233696	-0.285727	2.852054
30	1	0	-4.259775	-0.532699	1.412411
31	8	0	-1.673900	1.584861	-3.070042
32	1	0	-2.355676	0.903337	-3.262400
33	1	0	-2.086608	2.476056	-3.026867
34	1	0	2.634366	-1.809815	-0.427543

```
SCF Done:  E(RB3LYP) =  -934.677974779     A.U. after    1 cycles
Zero-point correction=                           0.275289 (Hartree/Particle)
 Thermal correction to Energy=                   0.294482
 Thermal correction to Enthalpy=                 0.295426
 Thermal correction to Gibbs Free Energy=        0.227546
 Sum of electronic and zero-point Energies=          -934.402686
 Sum of electronic and thermal Energies=             -934.383493
 Sum of electronic and thermal Enthalpies=           -934.382549
 Sum of electronic and thermal Free Energies=        -934.450429
SCF Done:  E(RB3LYP) =  -934.976229730     A.U. after   16 cycles
```

3M2+H++H2O HCCHwTS2pcm.for4.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.813537	-0.595489	0.000714
2	6	0	-1.953602	0.536795	0.254428
3	6	0	-0.629000	0.493370	0.027748
4	1	0	-0.161458	-0.416029	-0.335105
5	1	0	-2.435311	1.430577	0.632715
6	6	0	0.209141	1.699332	0.357136

7	8	0	-0.217772	2.527719	1.165655
8	7	0	1.425432	1.787306	-0.243985
9	6	0	1.887432	0.884122	-1.311533
10	1	0	2.501041	1.483549	-1.993389
11	1	0	1.034067	0.548781	-1.907652
12	6	0	2.657869	-0.261678	-0.813082
13	6	0	3.282712	-1.209561	-0.396231
14	1	0	3.845619	-2.054867	-0.029573
15	8	0	-2.287177	-1.711274	-0.399790
16	8	0	-4.072006	-0.415002	0.191771
17	6	0	-5.066130	-1.462972	-0.051876
18	1	0	-6.015019	-0.989789	0.184606
19	1	0	-4.881962	-2.302009	0.620985
20	1	0	-5.036660	-1.753068	-1.103673
21	6	0	2.346453	2.852755	0.146830
22	1	0	3.331620	2.421897	0.351387
23	1	0	1.963603	3.337703	1.042660
24	1	0	2.441423	3.592689	-0.656034
25	8	0	4.934204	-3.631432	0.730724
26	1	0	5.622495	-3.168758	1.235240
27	1	0	4.345129	-3.978090	1.419977
28	1	0	-2.918632	-2.443857	-0.545957

SCF Done: E(RB3LYP) = -706.755844921 A.U. after 1 cycles
Zero-point correction= 0.224796 (Hartree/Particle)
Thermal correction to Energy= 0.243554
Thermal correction to Enthalpy= 0.244498
Thermal correction to Gibbs Free Energy= 0.174680
Sum of electronic and zero-point Energies= -706.531049
Sum of electronic and thermal Energies= -706.512291
Sum of electronic and thermal Enthalpies= -706.511346
Sum of electronic and thermal Free Energies= -706.581165
SCF Done: E(RB3LYP) = -706.996237116 A.U. after 16 cycles

TS7 HCCHwTS2pcm.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.270099	-0.327030	-0.001697
2	6	0	0.997735	-0.791213	-0.292579
3	6	0	-0.086546	-0.557786	0.583055
4	1	0	0.158303	-0.335372	1.616952
5	1	0	0.855648	-1.282061	-1.247493
6	6	0	-1.284497	-1.499666	0.435560
7	8	0	-1.219330	-2.634558	0.895858
8	7	0	-2.317669	-0.968901	-0.252523
9	6	0	-2.216252	0.425126	-0.657996
10	1	0	-3.142015	0.956804	-0.412845
11	1	0	-2.050124	0.513500	-1.740133
12	6	0	-1.082141	1.025389	0.094406
13	6	0	-0.561362	2.052714	0.557287
14	1	0	0.122186	2.712971	1.047040
15	8	0	2.459186	0.403208	1.089460
16	8	0	3.254114	-0.600179	-0.835942
17	6	0	4.587763	-0.082708	-0.618572
18	1	0	5.165811	-0.438254	-1.468817
19	1	0	5.013706	-0.488006	0.303825
20	1	0	4.578675	1.010495	-0.611405
21	6	0	-3.507895	-1.733981	-0.587632
22	1	0	-4.393492	-1.287034	-0.123198
23	1	0	-3.372407	-2.748802	-0.213329
24	1	0	-3.649076	-1.758992	-1.673476
25	8	0	-1.613241	4.113952	-0.058756
26	1	0	-1.681258	4.011082	-1.022643
27	1	0	-2.522222	3.972810	0.254585
28	1	0	3.392691	0.618714	1.262664

SCF Done: E(RB3LYP) = -706.728580623 A.U. after 1 cycles
Zero-point correction= 0.224411 (Hartree/Particle)
Thermal correction to Energy= 0.241677
Thermal correction to Enthalpy= 0.242621
Thermal correction to Gibbs Free Energy= 0.178783

```
 Sum of electronic and zero-point Energies=           -706.504170
 Sum of electronic and thermal Energies=              -706.486904
 Sum of electronic and thermal Enthalpies=            -706.485960
 Sum of electronic and thermal Free Energies=         -706.549797
SCF Done:  E(RB3LYP) =  -706.965060602     A.U. after   15 cycles


CM4+H+         HCCHwTS2pcm.rev.log
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.264713   -0.451407    0.092608
      2          6           0        1.051892   -0.353394   -0.470912
      3          6           0       -0.216821   -0.263432    0.320320
      4          1           0        0.021992   -0.377261    1.387074
      5          1           0        0.992487   -0.360473   -1.553377
      6          6           0       -1.253303   -1.364561    0.001872
      7          8           0       -1.002531   -2.554113   -0.144294
      8          7           0       -2.487549   -0.791669   -0.049002
      9          6           0       -2.505797    0.650167    0.147748
     10          1           0       -2.991817    0.912590    1.099588
     11          1           0       -3.060015    1.145797   -0.659450
     12          6           0       -1.034272    1.008503    0.152559
     13          6           0       -0.464797    2.190448    0.003586
     14          1           0        0.581420    2.450489   -0.026251
     15          8           0        2.454828   -0.313238    1.436013
     16          8           0        3.370351   -0.704270   -0.651641
     17          6           0        4.468328    0.219057   -0.496413
     18          1           0        5.237146   -0.117558   -1.192019
     19          1           0        4.867608    0.207658    0.521910
     20          1           0        4.148873    1.234302   -0.755474
     21          6           0       -3.715653   -1.541366   -0.229505
     22          1           0       -4.367787   -1.435215    0.645312
     23          1           0       -3.449390   -2.591241   -0.358446
     24          1           0       -4.254883   -1.190039   -1.116480
     25          8           0       -1.262675    3.425281   -0.122494
     26          1           0       -1.438553    3.716027   -1.046388
     27          1           0       -2.088655    3.464827    0.406535
     28          1           0        3.168904   -0.911590    1.718630
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -706.772286704     A.U. after    1 cycles
Zero-point correction=                           0.230867 (Hartree/Particle)
 Thermal correction to Energy=                    0.246480
 Thermal correction to Enthalpy=                  0.247424
 Thermal correction to Gibbs Free Energy=         0.186953
 Sum of electronic and zero-point Energies=           -706.541419
 Sum of electronic and thermal Energies=              -706.525807
 Sum of electronic and thermal Enthalpies=            -706.524863
 Sum of electronic and thermal Free Energies=         -706.585333
SCF Done:  E(RB3LYP) =  -707.002812173     A.U. after   17 cycles


Scheme 16
6M3          diEMeCCTS3pcm.for.log
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.082804    0.902220   -0.098528
      2          6           0        1.107065   -0.246774   -0.170647
      3          6           0       -0.224084   -0.096946   -0.234314
      4          1           0       -0.824889   -0.996713   -0.312756
      5          6           0        1.671974   -1.633248   -0.231597
      6          6           0       -0.880908    1.242830   -0.129022
      7          8           0       -0.262155    2.202733    0.347382
      8          7           0       -2.174579    1.335061   -0.549216
      9          6           0       -2.904454    0.247324   -1.221433
     10          1           0       -2.211985   -0.326868   -1.843591
     11          1           0       -3.604756    0.720244   -1.919309
     12          6           0       -3.629309   -0.633773   -0.296560
     13          6           0       -4.215452   -1.361185    0.473390
     14          6           0       -4.925342   -2.238515    1.401937
```

15	8	0	1.005126	-2.649289	-0.273581
16	8	0	2.465771	1.521904	-1.068796
17	8	0	2.520473	1.084157	1.152273
18	6	0	3.485886	2.142552	1.330190
19	1	0	3.733414	2.133282	2.390876
20	1	0	3.047161	3.101983	1.046554
21	1	0	4.375365	1.951482	0.725610
22	8	0	3.013260	-1.607507	-0.238887
23	6	0	3.673486	-2.889779	-0.300905
24	1	0	4.739126	-2.665953	-0.303134
25	1	0	3.387367	-3.416574	-1.213841
26	1	0	3.407185	-3.492098	0.570410
27	6	0	-2.922213	2.568964	-0.323961
28	1	0	-3.135034	3.070946	-1.275064
29	1	0	-2.329297	3.228293	0.307061
30	1	0	-3.870333	2.336822	0.172648
31	1	0	-5.994681	-2.000142	1.435374
32	1	0	-4.528059	-2.138785	2.418673
33	1	0	-4.825056	-3.289346	1.106589

SCF Done: E(RB3LYP) = -897.129599284 A.U. after 1 cycles
Zero-point correction= 0.260397 (Hartree/Particle)
Thermal correction to Energy= 0.281445
Thermal correction to Enthalpy= 0.282389
Thermal correction to Gibbs Free Energy= 0.206601
Sum of electronic and zero-point Energies= -896.869203
Sum of electronic and thermal Energies= -896.848155
Sum of electronic and thermal Enthalpies= -896.847210
Sum of electronic and thermal Free Energies= -896.922998
SCF Done: E(RB3LYP) = -897.407712689 A.U. after 15 cycles

TS8 diEMeCCTS3pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.768326	1.422591	0.082221
2	6	0	0.815834	-0.042865	-0.086931
3	6	0	-0.424352	-0.784540	-0.244541
4	1	0	-0.191168	-1.748566	-0.711972
5	6	0	2.034566	-0.745275	-0.535610
6	6	0	-1.586149	-0.151172	-1.043426
7	8	0	-1.425949	0.535966	-2.044979
8	7	0	-2.779982	-0.559395	-0.542877
9	6	0	-2.719113	-1.377333	0.659484
10	1	0	-2.968288	-2.425782	0.440196
11	1	0	-3.420126	-1.011670	1.417144
12	6	0	-1.300175	-1.229501	1.119468
13	6	0	-0.605904	-1.269083	2.182867
14	6	0	0.645329	-0.910754	2.699329
15	8	0	2.040267	-1.900521	-0.950340
16	8	0	1.607745	2.243838	-0.246697
17	8	0	-0.393786	1.784328	0.696518
18	6	0	-0.605292	3.197207	0.846811
19	1	0	-1.571403	3.297027	1.341840
20	1	0	-0.625447	3.689822	-0.128960
21	1	0	0.183443	3.642556	1.458571
22	8	0	3.168817	-0.027963	-0.398136
23	6	0	4.377918	-0.697168	-0.793857
24	1	0	5.176061	0.026983	-0.629452
25	1	0	4.336042	-0.983339	-1.847959
26	1	0	4.543596	-1.590164	-0.185351
27	6	0	-4.049355	-0.279326	-1.187231
28	1	0	-4.539696	-1.210105	-1.495799
29	1	0	-3.852028	0.335139	-2.066181
30	1	0	-4.715891	0.260814	-0.505501
31	1	0	0.656235	-0.048188	3.372501
32	1	0	1.061848	-0.485750	1.654412
33	1	0	1.300146	-1.714886	3.044222

SCF Done: E(RB3LYP) = -897.090962350 A.U. after 1 cycles
Zero-point correction= 0.258107 (Hartree/Particle)
Thermal correction to Energy= 0.276814

```
 Thermal correction to Enthalpy=                  0.277759
 Thermal correction to Gibbs Free Energy=         0.210830
 Sum of electronic and zero-point Energies=           -896.832855
 Sum of electronic and thermal Energies=              -896.814148
 Sum of electronic and thermal Enthalpies=            -896.813204
 Sum of electronic and thermal Free Energies=         -896.880132
SCF Done:  E(RB3LYP) =  -897.366117586     A.U. after   17 cycles
```

10M1 diEMeCCTS3pcm.rev.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.799462	0.958853	0.995675
2	6	0	0.878965	-0.315979	0.148998
3	6	0	-0.402263	-0.597651	-0.671028
4	1	0	-0.078046	-1.017582	-1.633076
5	6	0	2.127099	-0.255706	-0.728470
6	6	0	-1.231327	0.646238	-1.025189
7	8	0	-0.771828	1.733125	-1.370588
8	7	0	-2.546240	0.329681	-0.915124
9	6	0	-2.813943	-1.014795	-0.417017
10	1	0	-3.278384	-1.632378	-1.199403
11	1	0	-3.500459	-0.983729	0.437273
12	6	0	-1.429037	-1.520711	-0.030180
13	6	0	-1.182379	-2.552131	0.731920
14	6	0	-0.922885	-3.575509	1.504616
15	8	0	2.131796	-0.059131	-1.926285
16	8	0	1.626074	1.846277	1.006693
17	8	0	-0.304494	0.943850	1.757105
18	6	0	-0.514163	2.105410	2.589131
19	1	0	-1.438770	1.910068	3.130602
20	1	0	-0.612756	2.998807	1.968528
21	1	0	0.319945	2.229071	3.283082
22	8	0	3.227523	-0.477217	0.002987
23	6	0	4.482945	-0.408538	-0.705219
24	1	0	5.248566	-0.617736	0.040755
25	1	0	4.623078	0.588062	-1.130080
26	1	0	4.509508	-1.154295	-1.502908
27	6	0	-3.620070	1.238055	-1.263969
28	1	0	-4.240268	0.815172	-2.063074
29	1	0	-3.174443	2.173002	-1.606672
30	1	0	-4.257251	1.435968	-0.393993
31	1	0	-0.832348	-3.468935	2.584862
32	1	0	1.020097	-1.144821	0.853578
33	1	0	-0.791792	-4.578890	1.101481

```
SCF Done:  E(RB3LYP) =  -897.160564856     A.U. after    1 cycles
Zero-point correction=                           0.262464 (Hartree/Particle)
 Thermal correction to Energy=                   0.281763
 Thermal correction to Enthalpy=                 0.282707
 Thermal correction to Gibbs Free Energy=        0.213417
 Sum of electronic and zero-point Energies=           -896.898101
 Sum of electronic and thermal Energies=              -896.878802
 Sum of electronic and thermal Enthalpies=            -896.877858
 Sum of electronic and thermal Free Energies=         -896.947148
SCF Done:  E(RB3LYP) =  -897.435421604     A.U. after   15 cycles
```

6M3+H2O diEMeCCwTS1pcm.for4.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.452853	-0.870375	-0.437682
2	6	0	-1.559730	0.290190	-0.079836
3	6	0	-0.231979	0.191128	0.084466
4	1	0	0.316698	1.106637	0.280384
5	6	0	-2.191767	1.643519	0.046810
6	6	0	0.501169	-1.103852	-0.072568
7	8	0	0.000744	-2.026860	-0.726554

8	7	0	1.734672	-1.191140	0.502858
9	6	0	2.298736	-0.161202	1.387964
10	1	0	2.921406	-0.678415	2.126509
11	1	0	1.495896	0.313293	1.959387
12	6	0	3.093438	0.858075	0.685402
13	6	0	3.722832	1.723879	0.116546
14	6	0	4.496563	2.755272	-0.573495
15	8	0	-1.573293	2.678878	0.204345
16	8	0	-2.942536	-1.016062	-1.538028
17	8	0	-2.681594	-1.660504	0.617726
18	6	0	-3.510984	-2.815046	0.365698
19	1	0	-3.615385	-3.312477	1.329059
20	1	0	-3.022704	-3.473950	-0.356167
21	1	0	-4.486567	-2.507637	-0.017265
22	8	0	-3.528724	1.563552	-0.013453
23	6	0	-4.245497	2.810298	0.111300
24	1	0	-5.299340	2.545721	0.039539
25	1	0	-3.962134	3.489186	-0.695961
26	1	0	-4.028359	3.274702	1.075733
27	6	0	2.565263	-2.371027	0.265726
28	1	0	3.557729	-2.062639	-0.080302
29	1	0	2.086518	-2.985111	-0.494817
30	1	0	2.672927	-2.955382	1.187260
31	8	0	5.609067	-0.791547	-0.849588
32	1	0	6.181962	-0.997589	-0.094050
33	1	0	4.943012	-0.194171	-0.465190
34	1	0	5.386366	2.322106	-1.043995
35	1	0	4.827981	3.529509	0.127490
36	1	0	3.900822	3.239393	-1.355180

SCF Done: E(RB3LYP) = -973.552445311 A.U. after 1 cycles
Zero-point correction= 0.284090 (Hartree/Particle)
Thermal correction to Energy= 0.308762
Thermal correction to Enthalpy= 0.309706
Thermal correction to Gibbs Free Energy= 0.224047
Sum of electronic and zero-point Energies= -973.268355
Sum of electronic and thermal Energies= -973.243683
Sum of electronic and thermal Enthalpies= -973.242739
Sum of electronic and thermal Free Energies= -973.328398
SCF Done: E(RB3LYP) = -973.875542430 A.U. after 15 cycles

TS9 diEMeCCwTS1pcm.log
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.027531	-1.374938	0.847791
2	6	0	-1.078212	-0.374758	-0.197637
3	6	0	0.110171	0.059410	-0.905473
4	1	0	-0.179312	0.647555	-1.776152
5	6	0	-2.280848	0.363932	-0.537262
6	6	0	1.124388	-1.018090	-1.342017
7	8	0	0.814401	-1.926331	-2.104857
8	7	0	2.361240	-0.789900	-0.839985
9	6	0	2.459426	0.288333	0.121805
10	1	0	3.337668	0.910388	-0.074654
11	1	0	2.523841	-0.097762	1.148173
12	6	0	1.197385	1.087599	-0.060004
13	6	0	0.842448	2.274673	0.167958
14	6	0	0.052588	3.475359	0.303934
15	8	0	-2.297553	1.335529	-1.304053
16	8	0	-1.955889	-1.914977	1.440646
17	8	0	0.277663	-1.699724	1.157540
18	6	0	0.443455	-2.734294	2.133512
19	1	0	1.520650	-2.873810	2.235254
20	1	0	-0.026999	-3.664915	1.803102
21	1	0	0.009814	-2.440081	3.093577
22	8	0	-3.424081	-0.075700	0.049114
23	6	0	-4.605264	0.672323	-0.268463
24	1	0	-5.412560	0.187884	0.282732
25	1	0	-4.812301	0.644480	-1.342012
26	1	0	-4.506848	1.715434	0.046139
27	6	0	3.469933	-1.702751	-1.040722

28	1	0	4.358721	-1.156874	-1.374727
29	1	0	3.175854	-2.423877	-1.804327
30	1	0	3.710409	-2.235686	-0.112221
31	8	0	2.762886	3.358546	1.344264
32	1	0	3.136635	2.792721	2.039334
33	1	0	3.497534	3.485565	0.722144
34	1	0	-0.068650	3.755925	1.354618
35	1	0	-0.940500	3.247538	-0.110747
36	1	0	0.480329	4.315290	-0.252099

```
SCF Done:  E(RB3LYP) =  -973.516254529     A.U. after    1 cycles
Zero-point correction=                           0.283196 (Hartree/Particle)
 Thermal correction to Energy=                    0.306078
 Thermal correction to Enthalpy=                  0.307022
 Thermal correction to Gibbs Free Energy=         0.230093
 Sum of electronic and zero-point Energies=           -973.233059
 Sum of electronic and thermal Energies=              -973.210176
 Sum of electronic and thermal Enthalpies=            -973.209232
 Sum of electronic and thermal Free Energies=         -973.286162
SCF Done:  E(RB3LYP) =  -973.836794254     A.U. after   17 cycles
```

CM5 diEMeCCwTS1pcm.rev.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.819412	-1.104510	1.088333
2	6	0	-0.976248	-0.333882	-0.102857
3	6	0	0.239910	0.165298	-0.853000
4	1	0	-0.149760	0.657999	-1.752282
5	6	0	-2.233421	0.053267	-0.657689
6	6	0	1.206710	-0.931837	-1.331661
7	8	0	0.896122	-1.927881	-1.978295
8	7	0	2.478503	-0.598799	-0.967423
9	6	0	2.578174	0.568137	-0.112011
10	1	0	3.320419	1.276332	-0.505676
11	1	0	2.892843	0.280770	0.903079
12	6	0	1.172448	1.133533	-0.126874
13	6	0	0.778144	2.298886	0.361269
14	6	0	-0.506926	3.036741	0.379854
15	8	0	-2.379907	0.818944	-1.631308
16	8	0	-1.664586	-1.602337	1.836769
17	8	0	0.536422	-1.266604	1.395875
18	6	0	0.810921	-2.034919	2.565592
19	1	0	1.899219	-2.075985	2.647611
20	1	0	0.406699	-3.048922	2.482165
21	1	0	0.388813	-1.566326	3.460762
22	8	0	-3.344967	-0.471173	-0.041759
23	6	0	-4.598183	-0.041550	-0.575728
24	1	0	-5.359685	-0.550007	0.019674
25	1	0	-4.703640	-0.318785	-1.629322
26	1	0	-4.722083	1.042946	-0.487727
27	6	0	3.629077	-1.440176	-1.219763
28	1	0	4.425864	-0.870303	-1.711630
29	1	0	3.309316	-2.254603	-1.871525
30	1	0	4.024452	-1.859130	-0.285184
31	8	0	1.827227	3.116235	1.115439
32	1	0	2.359650	2.608397	1.764870
33	1	0	2.426071	3.644173	0.542603
34	1	0	-0.913800	3.113817	1.394886
35	1	0	-1.223054	2.507056	-0.253668
36	1	0	-0.380504	4.052768	-0.013247

```
SCF Done:  E(RB3LYP) =  -973.534632959     A.U. after    1 cycles
Zero-point correction=                           0.288848 (Hartree/Particle)
 Thermal correction to Energy=                    0.309997
 Thermal correction to Enthalpy=                  0.310941
 Thermal correction to Gibbs Free Energy=         0.239102
 Sum of electronic and zero-point Energies=           -973.245785
 Sum of electronic and thermal Energies=              -973.224636
 Sum of electronic and thermal Enthalpies=            -973.223692
 Sum of electronic and thermal Free Energies=         -973.295531
SCF Done:  E(RB3LYP) =  -973.851534617     A.U. after   16 cycles
```

3M3 MeCCTS4pcm.for3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.062895	-1.652637	-0.528691
2	6	0	1.728565	-0.689271	-0.158793
3	6	0	0.431567	-0.452645	0.071636
4	1	0	0.131455	0.528039	0.424752
5	6	0	2.750584	0.359372	0.077981
6	6	0	-0.592082	-1.509820	-0.208135
7	8	0	-0.300548	-2.501762	-0.886586
8	7	0	-1.846329	-1.314057	0.299224
9	6	0	-2.215740	-0.207147	1.195278
10	1	0	-1.373204	0.031199	1.850249
11	1	0	-3.004555	-0.583654	1.856721
12	6	0	-2.682392	0.993675	0.488671
13	6	0	-3.058502	1.982340	-0.100115
14	6	0	-3.512476	3.175755	-0.811378
15	8	0	2.527824	1.487260	0.483301
16	8	0	3.980522	-0.101453	-0.218102
17	6	0	5.063564	0.829936	-0.029632
18	1	0	5.965644	0.289625	-0.314241
19	1	0	5.117563	1.143675	1.015675
20	1	0	4.924944	1.707654	-0.665545
21	6	0	-2.924611	-2.226610	-0.068582
22	1	0	-3.250477	-2.811772	0.799712
23	1	0	-2.563033	-2.901270	-0.842198
24	1	0	-3.778325	-1.654060	-0.447278
25	1	0	-4.598741	3.298204	-0.730581
26	1	0	-3.260827	3.117949	-1.876745
27	1	0	-3.042288	4.079585	-0.406888

SCF Done: E(RB3LYP) = -669.259870858 A.U. after 1 cycles
Zero-point correction= 0.217701 (Hartree/Particle)
Thermal correction to Energy= 0.234207
Thermal correction to Enthalpy= 0.235151
Thermal correction to Gibbs Free Energy= 0.169710
Sum of electronic and zero-point Energies= -669.042170
Sum of electronic and thermal Energies= -669.025664
Sum of electronic and thermal Enthalpies= -669.024719
Sum of electronic and thermal Free Energies= -669.090161
SCF Done: E(RB3LYP) = -669.467444376 A.U. after 15 cycles

TS10 MeCCTS4pcm.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.877635	-0.518471	-1.531520
2	6	0	0.881230	-0.213822	-0.489512
3	6	0	-0.334520	-0.145492	0.235645
4	1	0	-0.170659	-0.228552	1.315242
5	6	0	2.140849	-0.345942	0.242913
6	6	0	-1.531272	-1.002560	-0.196398
7	8	0	-1.421775	-2.123573	-0.685804
8	7	0	-2.708920	-0.396167	0.111326
9	6	0	-2.622370	0.975249	0.602674
10	1	0	-2.788511	1.017671	1.689413
11	1	0	-3.382409	1.598957	0.120116
12	6	0	-1.250610	1.420966	0.227822
13	6	0	-0.547080	2.387880	-0.177043
14	6	0	0.723085	2.645375	-0.726669
15	8	0	2.290914	-0.189139	1.449325
16	8	0	3.167291	-0.662772	-0.588384
17	6	0	4.453907	-0.800703	0.034826
18	1	0	5.145161	-1.047999	-0.771194
19	1	0	4.439903	-1.600502	0.780189

20	1	0	4.753086	0.133629	0.517667
21	6	0	-3.995666	-1.054760	-0.009675
22	1	0	-4.494288	-1.108830	0.965372
23	1	0	-3.824952	-2.063642	-0.386257
24	1	0	-4.644792	-0.510728	-0.705713
25	1	0	0.731879	2.983855	-1.767149
26	1	0	1.102058	1.502058	-0.760395
27	1	0	1.421567	3.222448	-0.113651

```
SCF Done:  E(RB3LYP) =  -669.212022664     A.U. after    1 cycles
Zero-point correction=                           0.215009 (Hartree/Particle)
 Thermal correction to Energy=                    0.229331
 Thermal correction to Enthalpy=                  0.230275
 Thermal correction to Gibbs Free Energy=         0.173360
 Sum of electronic and zero-point Energies=           -668.997013
 Sum of electronic and thermal Energies=              -668.982692
 Sum of electronic and thermal Enthalpies=            -668.981748
 Sum of electronic and thermal Free Energies=         -669.038662
SCF Done:  E(RB3LYP) =  -669.417976978     A.U. after   15 cycles
```

```
10M2         MeCCTS4pcm.rev.log
                         Standard orientation:
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.576626	-2.043478	-0.438262
2	6	0	0.703477	-0.952518	-0.431050
3	6	0	-0.448847	-0.346996	0.371278
4	1	0	-0.248269	-0.536663	1.436229
5	6	0	2.060515	-0.663749	0.179108
6	6	0	-1.794388	-1.013956	0.053936
7	8	0	-1.975736	-2.224571	-0.064845
8	7	0	-2.744102	-0.047624	-0.047658
9	6	0	-2.251709	1.313752	0.129885
10	1	0	-2.633972	1.742656	1.068166
11	1	0	-2.582166	1.959581	-0.692123
12	6	0	-0.737723	1.130828	0.152491
13	6	0	0.138493	2.081487	-0.035005
14	6	0	1.015903	3.033345	-0.222782
15	8	0	2.268543	-0.465698	1.361173
16	8	0	3.029639	-0.696276	-0.752094
17	6	0	4.374287	-0.496073	-0.270932
18	1	0	5.011829	-0.563327	-1.151789
19	1	0	4.639536	-1.269119	0.454105
20	1	0	4.467841	0.487561	0.195396
21	6	0	-4.152284	-0.324525	-0.246378
22	1	0	-4.741611	0.021875	0.611348
23	1	0	-4.272469	-1.403219	-0.356437
24	1	0	-4.519976	0.177643	-1.148775
25	1	0	1.378893	3.291567	-1.216949
26	1	0	0.687618	-0.620255	-1.472371
27	1	0	1.418917	3.611339	0.607880

```
SCF Done:  E(RB3LYP) =  -669.293527296     A.U. after    1 cycles
Zero-point correction=                           0.219586 (Hartree/Particle)
 Thermal correction to Energy=                    0.234388
 Thermal correction to Enthalpy=                  0.235332
 Thermal correction to Gibbs Free Energy=         0.176317
 Sum of electronic and zero-point Energies=           -669.073941
 Sum of electronic and thermal Energies=              -669.059139
 Sum of electronic and thermal Enthalpies=            -669.058195
 Sum of electronic and thermal Free Energies=         -669.117210
SCF Done:  E(RB3LYP) =  -669.498225314     A.U. after   14 cycles
```