Electronic Supplementary Material (ESI) for Chemical Science.

Kinetic Hydricity of Silane Hydrides in the Gas Phase

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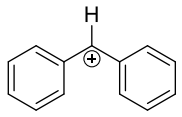
Calculated Structures

Calculated Structures of Electrophiles: Enthalpy (Free Energy) in Hartree, B3LYP/6-31+G(d), 298K



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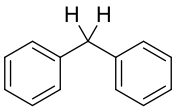

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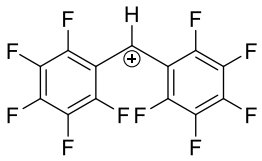

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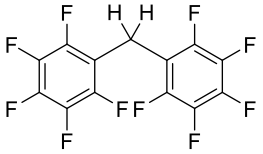

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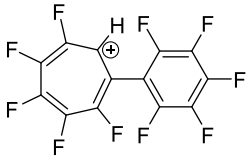

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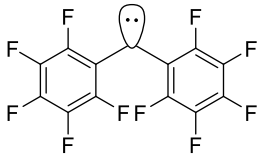

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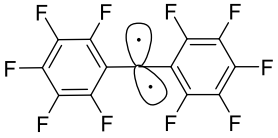

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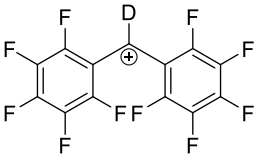

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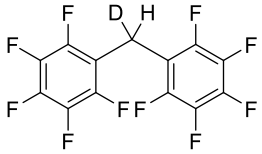

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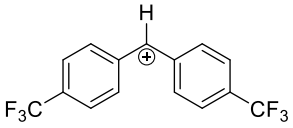

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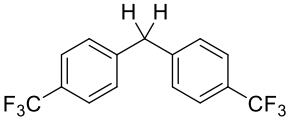

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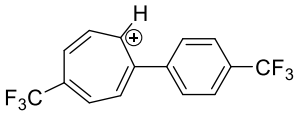

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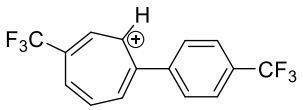

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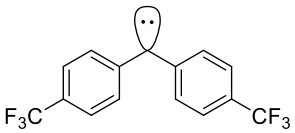

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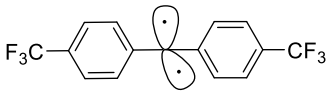

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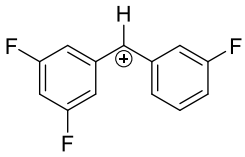

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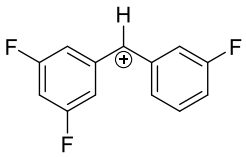

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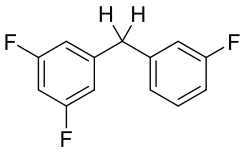

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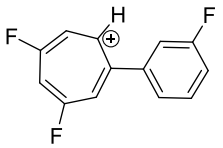

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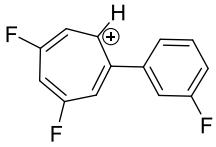

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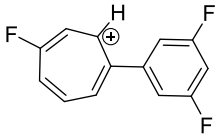

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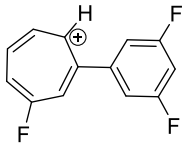

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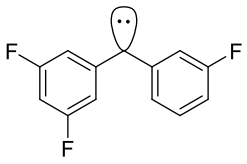

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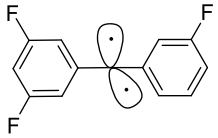

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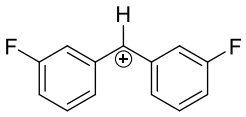

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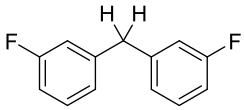

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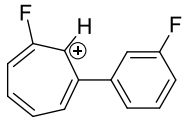

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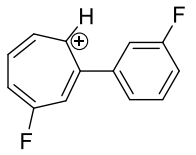

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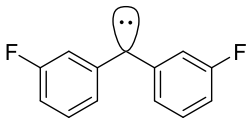

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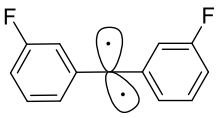

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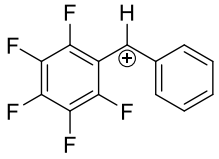

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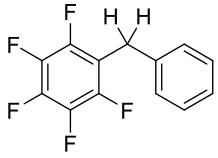

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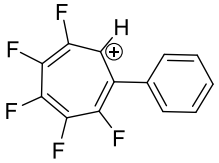

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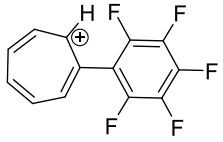

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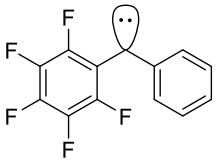

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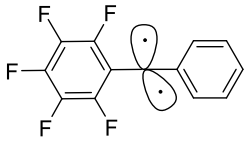

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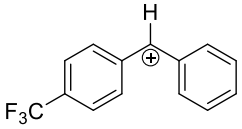

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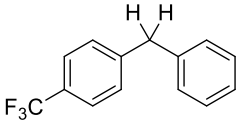

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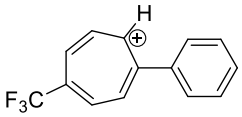

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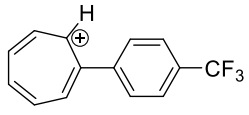
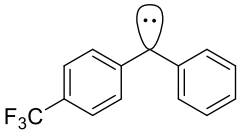
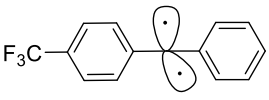
(-838.638176)
amarel/aek119/home/SiH/20074.log



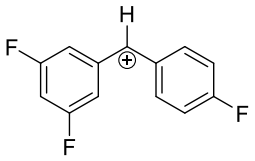
1f+_tropylium_2
-838.588479
(-838.646693)
amarel/aek119/home/SiH/20075-v2.log



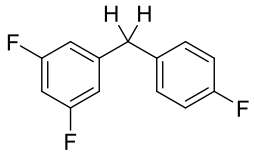
1f_carbene_s
-838.171639
(-838.230244)
amarel/aek119/home/SiH/20063s-v2.log



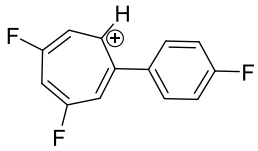
1f_carbene_t
-838.181278
(-838.241954)
amarel/aek/home/SiH/20063t.log



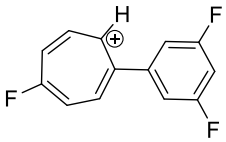
1g+
-799.284265
(-799.337905)
amarel/aek119/home/SiH/10745.log



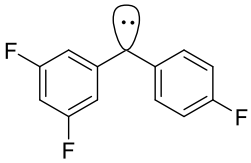
1gH
-800.160383
(-800.216385)
amarel/aek119/home/SiH/10755.log



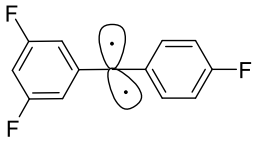
1g+_tropylium_1
-799.278089
(-799.331196)
amarel/jx112/home/prf/1i_1.log



1g+_tropylium_2
-799.281053
(-799.334024)
amarel/jx112/home/prf/1i_2.log

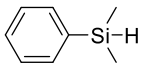


1g_carbene_s
-798.867323
(-798.921156)
amarel/aek119/home/SiH/11234s-v2.log

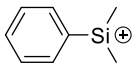


1g_carbene_t
-798.874885
(-798.930797)
amarel/aek/home/SiH/11234t.log

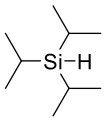
Calculated Structures of Silane Hydrides: Enthalpy (Free Energy) in Hartree, B3LYP/6-31+G(d), 298K



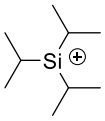
2
-601.426263
(-601.474541)
amarel/aek119/home/SiH/11093.log



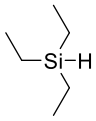
2+
-600.566312
(-600.615147)
amarel/aek119/home/SiH/11194.log



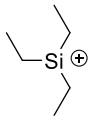
3
-645.427584
(-645.485566)
amarel/aek119/home/SiH/11092-v2.log



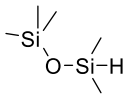
3+
-644.564522
(-644.625603)
amarel/aek119/home/SiH/11195-v2log



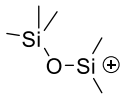
4
-527.583593
(-527.634286)
fen2/yn81/home/Notebook_2/209008.log



4+
-526.714786
(-526.766500)
amarel/aek119/home/SiH/11192-v2.log



5
-854.330901
(-854.391204)
amarel/aek119/home/SiH/11094-v4.log



5+
-853.472965
(-853.533144)
amarel/aek119/home/SiH/11193-v2.log

TMS
-409.743653
(-409.781434)
amarel/aek119/home/SiH/11103.log

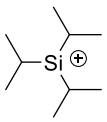
TMS+
-408.867156
(-408.908670)
amarel/aek119/home/SiH/11112-v2.log

H-
-0.459456
(-0.471816)
amarel/aek119/home/SiH/H-.log

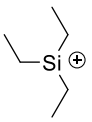
H_2

H_2
-1.162033
(-1.176825)
amarel/aek119/home/SiH/H2.log

Calculated Structures of Silane Hydrides: Enthalpy (Free Energy) in Hartree, B3LYP/6-31+G(d), scrf=(smd,solvent=methylene chloride), 298K

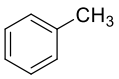


3+_smd(CH2Cl2)
-644.646124
(-644.704179)
amarel/aek119/home/SiH/3+_smd(CH2Cl2).log

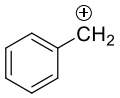


4+_smd(CH2Cl2)
-526.799060
(-526.849092)
amarel/aek119/home/SiH/4+_smd(CH2Cl2).log

Calculated Structures of Table 4 Reactions: Enthalpy (Free Energy) in Hartree, B3LYP/6-31+G(d), 298K

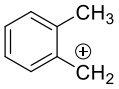


toluene
-271.442102
(-271.480127)
amarel/aek119/home/SiH/11200.log

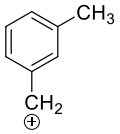


benzyl-cation
-270.542638
(-270.578378)
amarel/aek119/home/SiH/11201.log

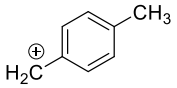
benzene
-232.153031
(-232.185843)
amarel/aek119/home/SiH/11202.log



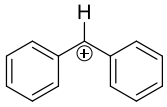
o-tolCH$_2$+
-309.837554
(-309.877221)
amarel/aek119/home/SiH/12203_o.log



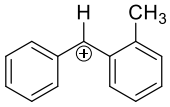
m-tolCH$_2$+
-309.836975
(-309.876928)
amarel/aek119/home/SiH/12203_m.log



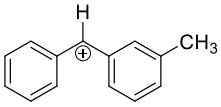
p-tolCH$_2$+
-309.843430
(-309.884269)
amarel/aek119/home/SiH/12203-v2_p.log



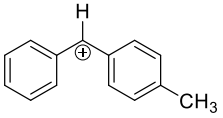
1+
-501.553785
(-501.601149)
amarel/aek119/home/SiH/11083.log



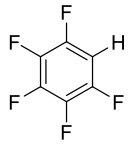
o-CH$_3$Ph$_2$CH+
-540.843933
(-540.894751)
amarel/aek119/home/SiH/11205_o.log



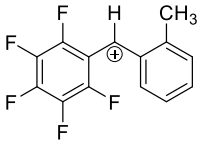
m-CH$_3$Ph$_2$CH+
-540.846126
(-540.897891)
amarel/aek119/home/SiH/11205_m.log



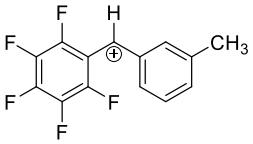
p-CH$_3$Ph$_2$CH+
-540.849757
(-540.902992)
amarel/aek119/home/SiH/11205_p.log



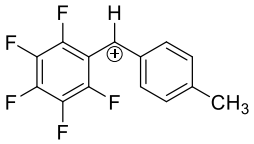
C$_6$F$_5$H
-728.362866
(-728.406395)
amarel/aek119/home/SiH/11214.log



o-CH$_3$Ph$_2$CHF$_5$+
-1037.028105
(-1037.089506)
amarel/aek119/home/SiH/11215_o.log



m-CH$_3$Ph$_2$CHF$_5$+
-1037.030010
(-1037.092326)
amarel/aek119/home/SiH/11215_m.log



p-CH$_3$Ph$_2$CHF$_5$+
-1037.034763
(-1037.098379)
amarel/aek119/home/SiH/11215_p.log

Detailed Coordinates Information

1+.log

SCF Done: E(RB3LYP) = -501.764426403 A.U. after 1 cycles

Zero-point correction= 0.199756
(Hartree/Particle)
Thermal correction to Energy= 0.209752
Thermal correction to Enthalpy= 0.210696
Thermal correction to Gibbs Free Energy= 0.163394
Sum of electronic and zero-point Energies= -501.564671
Sum of electronic and thermal Energies= -501.554674
Sum of electronic and thermal Enthalpies= -501.553730
Sum of electronic and thermal Free Energies= -501.601032

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	131.621	40.246	99.555

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.688206	-0.770388	-0.305626
2	6	0	2.395252	-1.267522	-0.280249
3	6	0	1.292624	-0.417236	0.036345
4	6	0	1.558510	0.935615	0.404147
5	6	0	2.857000	1.415111	0.400774
6	6	0	3.919414	0.571270	0.031590
7	1	0	4.518223	-1.417724	-0.570456
8	1	0	2.206800	-2.308014	-0.531336
9	1	0	0.753981	1.572898	0.751819
10	1	0	3.059067	2.438124	0.702607
11	1	0	4.934893	0.957737	0.031655
12	6	0	0.000013	-0.999508	-0.000197
13	1	0	0.000026	-2.090115	-0.000277
14	6	0	-1.292634	-0.417257	-0.036522
15	6	0	-1.558571	0.935579	-0.404313
16	6	0	-2.395193	-1.267540	0.280275
17	6	0	-2.857070	1.415065	-0.400777
18	1	0	-0.754090	1.572844	-0.752130
19	6	0	-3.688139	-0.770394	0.305883
20	1	0	-2.206697	-2.308030	0.531340
21	6	0	-3.919415	0.571245	-0.031364
22	1	0	-3.059189	2.438056	-0.702654
23	1	0	-4.518102	-1.417721	0.570906
24	1	0	-4.934894	0.957710	-0.031272

1H.log

SCF Done: E(RB3LYP) = -502.633957229 A.U. after 1 cycles

Zero-point correction= 0.209862
(Hartree/Particle)
Thermal correction to Energy= 0.220249
Thermal correction to Enthalpy= 0.221193
Thermal correction to Gibbs Free Energy= 0.170807
Sum of electronic and zero-point Energies= -502.424095
Sum of electronic and thermal Energies= -502.413708
Sum of electronic and thermal Enthalpies= -502.412764
Sum of electronic and thermal Free Energies= -502.463150

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.208	41.184	106.047

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.464438	0.857393	0.060591
2	6	0	2.276300	0.901613	0.798556
3	6	0	1.280647	-0.067998	0.622516
4	6	0	1.502050	-1.087612	-0.316926
5	6	0	2.686056	-1.137648	-1.054117
6	6	0	3.673331	-0.163352	-0.868584
7	1	0	4.223327	1.620986	0.213618
8	1	0	2.123702	1.699575	1.522855
9	1	0	0.736777	-1.844502	-0.475521
10	1	0	2.838702	-1.936900	-1.775467
11	1	0	4.594954	-0.201334	-1.443821
12	6	0	-0.000341	-0.029991	1.442406
13	1	0	-0.045213	-0.919462	2.085029
14	1	0	0.044021	0.831993	2.121544
15	6	0	-1.280825	0.042034	0.623829
16	6	0	-2.279779	-0.929968	0.764633
17	6	0	-1.498728	1.095838	-0.277907
18	6	0	-3.467661	-0.855038	0.028775
19	1	0	-2.130003	-1.754203	1.459488
20	6	0	-2.682452	1.176481	-1.012887
21	1	0	-0.730854	1.855374	-0.408713
22	6	0	-3.672989	0.199363	-0.862817
23	1	0	-4.229110	-1.621160	0.153911

24	1	0	-2.832256	2.001783	-1.704896
25	1	0	-4.594325	0.261170	-1.436447

1a+.log

SCF Done: E(RB3LYP) = -1494.05607015 A.U. after 1 cycles

Zero-point correction= 0.116993
(Hartree/Particle)
Thermal correction to Energy= 0.135957
Thermal correction to Enthalpy= 0.136901
Thermal correction to Gibbs Free Energy= 0.069251
Sum of electronic and zero-point Energies= -1493.939077
Sum of electronic and thermal Energies= -1493.920113
Sum of electronic and thermal Enthalpies= -1493.919169
Sum of electronic and thermal Free Energies= -1493.986819

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.314	69.857	142.381

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.957167	0.418297	-0.119385
2	6	0	2.917264	1.242110	-0.585771
3	6	0	1.613131	0.787721	-0.532836
4	6	0	1.287687	-0.505439	-0.017019
5	6	0	2.390188	-1.325105	0.391417
6	6	0	3.694856	-0.872155	0.371166
7	6	0	0.000143	-1.085379	-0.000543
8	1	0	0.000210	-2.173689	-0.000739
9	6	0	-1.287557	-0.505265	0.016534
10	6	0	-1.613020	0.787751	0.532607
11	6	0	-2.390343	-1.324970	-0.391603
12	6	0	-2.917166	1.242175	0.585509
13	6	0	-3.695034	-0.872107	-0.371051
14	6	0	-3.957254	0.418428	0.119408
15	9	0	-3.204146	2.429517	1.098612
16	9	0	-0.665764	1.541775	1.075737
17	9	0	-5.193023	0.855699	0.160743
18	9	0	-4.693682	-1.630622	-0.796441
19	9	0	-2.143311	-2.544367	-0.855522
20	9	0	0.665898	1.542071	-1.075683
21	9	0	3.204312	2.429529	-1.098568

22	9	0	5.193014	0.855469	-0.160257
23	9	0	4.693459	-1.630486	0.797011
24	9	0	2.143179	-2.544439	0.855495

1aH.log

SCF Done: E(RB3LYP) = -1494.97821325 A.U. after 1 cycles

Zero-point correction= 0.128088
(Hartree/Particle)
Thermal correction to Energy= 0.147474
Thermal correction to Enthalpy= 0.148419
Thermal correction to Gibbs Free Energy= 0.078860
Sum of electronic and zero-point Energies= -1494.850125
Sum of electronic and thermal Energies= -1494.830739
Sum of electronic and thermal Enthalpies= -1494.829795
Sum of electronic and thermal Free Energies= -1494.899353

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	92.542	71.085	146.398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.676140	-1.340144	-0.730740
2	6	0	1.518522	-1.215794	0.031742
3	6	0	1.269375	-0.108831	0.847173
4	6	0	2.254651	0.880833	0.870696
5	6	0	3.425538	0.785374	0.120775
6	6	0	3.635616	-0.330231	-0.685714
7	6	0	0.000013	0.000143	1.674480
8	6	0	-1.269360	0.108991	0.847167
9	6	0	-2.254539	-0.880769	0.870761
10	6	0	-1.518599	1.215888	0.031674
11	6	0	-3.425455	-0.785426	0.120866
12	6	0	-2.676245	1.340119	-0.730781
13	6	0	-3.635634	0.330122	-0.685665
14	9	0	0.611651	-2.211289	-0.024160
15	9	0	2.875093	-2.419744	-1.499103
16	9	0	4.754741	-0.434725	-1.410774
17	9	0	4.346995	1.756674	0.171956
18	9	0	2.093737	1.972013	1.643127
19	9	0	-0.611794	2.211433	-0.024300
20	9	0	-2.875308	2.419647	-1.499199

21	9	0	-4.754796	0.434484	-1.410701
22	9	0	-4.346844	-1.756794	0.172093
23	9	0	-2.093492	-1.971922	1.643190
24	1	0	-0.083884	-0.875881	2.323152
25	1	0	0.083905	0.876233	2.323065

1aH_tropylium.log

SCF Done: E(RB3LYP) = -1494.05501739 A.U. after 2 cycles

Zero-point correction= 0.117225
(Hartree/Particle)
Thermal correction to Energy= 0.135990
Thermal correction to Enthalpy= 0.136934
Thermal correction to Gibbs Free Energy= 0.069824
Sum of electronic and zero-point Energies= -1493.937792
Sum of electronic and thermal Energies= -1493.919028
Sum of electronic and thermal Enthalpies= -1493.918084
Sum of electronic and thermal Free Energies= -1493.985193

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	85.335	69.411	141.245

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.465151	-1.321708	-0.557899
2	6	0	-1.094035	-1.041278	-0.483187
3	6	0	-1.064194	1.253383	0.497302
4	6	0	-2.414500	1.557343	0.624160
5	6	0	-3.546988	0.771644	0.342412
6	6	0	-3.560454	-0.522721	-0.181817
7	6	0	-0.424378	0.097221	0.023298
8	6	0	1.055132	0.080332	0.028374
9	6	0	1.795108	1.135407	-0.537424
10	6	0	1.780303	-0.971870	0.617060
11	6	0	3.184306	1.137774	-0.540819
12	6	0	3.169631	-0.981341	0.639898
13	6	0	3.873563	0.074701	0.052285
14	1	0	-0.418792	2.054194	0.847225
15	9	0	1.149854	2.153864	-1.127318
16	9	0	3.855311	2.135288	-1.106215
17	9	0	5.195317	0.072364	0.063602
18	9	0	3.826716	-1.976445	1.224805

19	9	0	1.120927	-1.967542	1.221961
20	9	0	-0.342036	-2.002078	-0.994087
21	9	0	-2.786564	-2.490585	-1.075182
22	9	0	-4.747290	-1.060442	-0.366749
23	9	0	-4.720845	1.307562	0.598424
24	9	0	-2.697085	2.753847	1.117528

1a_carbene_s.log

SCF Done: E(RB3LYP) = -1493.64935037 A.U. after 1 cycles

Zero-point correction= 0.102301
(Hartree/Particle)
Thermal correction to Energy= 0.121489
Thermal correction to Enthalpy= 0.122433
Thermal correction to Gibbs Free Energy= 0.053931
Sum of electronic and zero-point Energies= -1493.547049
Sum of electronic and thermal Energies= -1493.527862
Sum of electronic and thermal Enthalpies= -1493.526917
Sum of electronic and thermal Free Energies= -1493.595420

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.235	70.039	144.175

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.853807	-1.102619	-0.837325
2	6	0	1.559659	-0.631392	-0.686994
3	6	0	1.254078	0.572823	0.011639
4	6	0	2.374596	1.241669	0.589122
5	6	0	3.664827	0.741712	0.510627
6	6	0	3.908217	-0.424692	-0.219750
7	6	0	-0.000012	1.241163	-0.000032
8	6	0	-1.254093	0.572777	-0.011796
9	6	0	-1.559595	-0.631373	0.686897
10	6	0	-2.374639	1.241630	-0.589132
11	6	0	-2.853733	-1.102640	0.837294
12	6	0	-3.664863	0.741640	-0.510607
13	6	0	-3.908191	-0.424748	0.219786
14	9	0	0.580198	-1.320272	-1.288340
15	9	0	3.105481	-2.216049	-1.538545
16	9	0	5.150220	-0.892276	-0.328506
17	9	0	4.687316	1.377860	1.095776

18	9	0	2.187199	2.372163	1.266997
19	9	0	-2.187387	2.372192	-1.266980
20	9	0	-4.687391	1.377799	-1.095712
21	9	0	-5.150206	-0.892359	0.328667
22	9	0	-3.105323	-2.216060	1.538563
23	9	0	-0.580144	-1.320298	1.288262

1a_carbene_t.log

SCF Done: E(UB3LYP) = -1493.66069607 A.U. after 1 cycles

Zero-point correction= 0.101462
(Hartree/Particle)
Thermal correction to Energy= 0.120991
Thermal correction to Enthalpy= 0.121935
Thermal correction to Gibbs Free Energy= 0.050911
Sum of electronic and zero-point Energies= -1493.559235
Sum of electronic and thermal Energies= -1493.539705
Sum of electronic and thermal Enthalpies= -1493.538761
Sum of electronic and thermal Free Energies= -1493.609785

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.923	70.738	149.483

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.084782	-1.113376	0.770316
2	6	0	1.755016	-0.732891	0.712068
3	6	0	1.328248	0.439887	0.024308
4	6	0	2.357506	1.209644	-0.587125
5	6	0	3.690639	0.839276	-0.529915
6	6	0	4.060556	-0.325819	0.150064
7	6	0	0.000004	0.856597	-0.000085
8	6	0	-1.328240	0.439845	-0.024354
9	6	0	-2.357444	1.209635	0.587103
10	6	0	-1.755056	-0.732906	-0.712095
11	6	0	-3.690588	0.839299	0.529934
12	6	0	-3.084837	-1.113374	-0.770304
13	6	0	-4.060570	-0.325770	-0.150053
14	9	0	0.837759	-1.494154	1.327365
15	9	0	3.449094	-2.225072	1.422579
16	9	0	5.344739	-0.687089	0.206543
17	9	0	4.631440	1.583911	-1.124763

18	9	0	2.025502	2.325685	-1.249912
19	9	0	-0.837846	-1.494221	-1.327400
20	9	0	-3.449172	-2.225066	-1.422545
21	9	0	-5.344767	-0.686982	-0.206484
22	9	0	-4.631355	1.583958	1.124817
23	9	0	-2.025404	2.325663	1.249894

1a-D+.log

SCF Done: E(RB3LYP) = -1494.05607034 A.U. after 1 cycles

Zero-point correction= 0.113624
(Hartree/Particle)
Thermal correction to Energy= 0.132730
Thermal correction to Enthalpy= 0.133674
Thermal correction to Gibbs Free Energy= 0.065786
Sum of electronic and zero-point Energies= -1493.942446
Sum of electronic and thermal Energies= -1493.923340
Sum of electronic and thermal Enthalpies= -1493.922396
Sum of electronic and thermal Free Energies= -1493.990284

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	83.289	70.535	142.882

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.916872	-1.242266	0.585332
2	6	0	1.612734	-0.787756	0.532352
3	6	0	1.287551	0.505463	0.016454
4	6	0	2.390266	1.325075	-0.391526
5	6	0	3.694926	0.872073	-0.370914
6	6	0	3.956997	-0.418592	0.119287
7	6	0	-0.000009	1.085653	0.000038
8	1	0	-0.000023	2.174079	0.000033
9	6	0	-1.287534	0.505492	-0.016403
10	6	0	-2.390313	1.325061	0.391531
11	6	0	-1.612699	-0.787732	-0.532351
12	6	0	-3.694961	0.872016	0.370910
13	6	0	-2.916819	-1.242256	-0.585334
14	6	0	-3.957020	-0.418653	-0.119300
15	9	0	2.143222	2.544669	-0.854890
16	9	0	4.693668	1.630499	-0.796147
17	9	0	5.192713	-0.855987	0.160369

18	9	0	3.203651	-2.429651	1.098388
19	9	0	0.665360	-1.541487	1.075586
20	9	0	-2.143358	2.544679	0.854888
21	9	0	-4.693708	1.630433	0.796165
22	9	0	-5.192700	-0.856061	-0.160446
23	9	0	-3.203566	-2.429661	-1.098413
24	9	0	-0.665272	-1.541382	-1.075553

1aH-D.log

SCF Done: E(RB3LYP) = -1494.97821324 A.U. after 1 cycles

Zero-point correction= 0.124664
(Hartree/Particle)
Thermal correction to Energy= 0.144177
Thermal correction to Enthalpy= 0.145121
Thermal correction to Gibbs Free Energy= 0.075349
Sum of electronic and zero-point Energies= -1494.853549
Sum of electronic and thermal Energies= -1494.834037
Sum of electronic and thermal Enthalpies= -1494.833092
Sum of electronic and thermal Free Energies= -1494.902864

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	90.472	71.707	146.847

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.675931	1.340371	-0.730410
2	6	0	-1.518470	1.215895	0.032284
3	6	0	-1.269368	0.108644	0.847340
4	6	0	-2.254540	-0.881133	0.870380
5	6	0	-3.425277	-0.785545	0.120221
6	6	0	-3.635287	0.330305	-0.685939
7	6	0	-0.000058	-0.000543	1.674742
8	1	0	0.083836	0.875253	2.323689
9	1	0	-0.083980	-0.876832	2.323033
10	6	0	1.269283	-0.109159	0.847322
11	6	0	2.254168	0.880880	0.870604
12	6	0	1.518742	-1.216201	0.032066
13	6	0	3.425000	0.785740	0.120512
14	6	0	2.676302	-1.340240	-0.730531
15	6	0	3.635393	-0.329919	-0.685789
16	9	0	-2.093708	-1.972484	1.642569

17	9	0	-4.346671	-1.756936	0.170919
18	9	0	-4.754284	0.434938	-1.411197
19	9	0	-2.874899	2.420221	-1.498415
20	9	0	-0.611692	2.211512	-0.023035
21	9	0	0.612196	-2.212007	-0.023533
22	9	0	2.875620	-2.419873	-1.498741
23	9	0	4.754455	-0.434123	-1.411014
24	9	0	4.346090	1.757411	0.171416
25	9	0	2.092936	1.972119	1.642861

1b+.log

SCF Done: E(RB3LYP) = -1175.85804880 A.U. after 1 cycles

Zero-point correction= 0.208080
(Hartree/Particle)
Thermal correction to Energy= 0.225529
Thermal correction to Enthalpy= 0.226473
Thermal correction to Gibbs Free Energy= 0.157165
Sum of electronic and zero-point Energies= -1175.649969
Sum of electronic and thermal Energies= -1175.632520
Sum of electronic and thermal Enthalpies= -1175.631576
Sum of electronic and thermal Free Energies= -1175.700884

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	141.521	65.782	145.872

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.854990	-0.866094	-0.388027
2	6	0	-1.559561	-0.384925	-0.399067
3	6	0	-1.292767	0.967861	-0.032004
4	6	0	-2.392920	1.815118	0.291432
5	6	0	-3.687390	1.318904	0.327357
6	6	0	-3.915275	-0.021260	-0.008412
7	1	0	-3.060358	-1.889064	-0.687465
8	1	0	-0.759653	-1.024577	-0.752527
9	1	0	-2.209033	2.856191	0.542276
10	1	0	-4.516297	1.962585	0.599822
11	6	0	0.000009	1.552625	0.000004
12	1	0	0.000002	2.643118	-0.000033
13	6	0	1.292789	0.967879	0.032042
14	6	0	2.392923	1.815137	-0.291434

15	6	0	1.559605	-0.384891	0.399175
16	6	0	3.687404	1.318938	-0.327364
17	1	0	2.209021	2.856200	-0.542306
18	6	0	2.855034	-0.866041	0.388125
19	1	0	0.759710	-1.024529	0.752690
20	6	0	3.915304	-0.021204	0.008436
21	1	0	4.516303	1.962622	-0.599853
22	1	0	3.060434	-1.888988	0.687620
23	6	0	5.324065	-0.595011	0.006806
24	6	0	-5.324076	-0.594999	-0.006836
25	9	0	-5.387579	-1.670665	0.805799
26	9	0	-5.665166	-0.996163	-1.249495
27	9	0	-6.234113	0.301003	0.410294
28	9	0	6.234205	0.301168	-0.409677
29	9	0	5.387621	-1.670234	-0.806421
30	9	0	5.664913	-0.996862	1.249320

1bH.log

SCF Done: E(RB3LYP) = -1176.75526665 A.U. after 1 cycles

Zero-point correction= 0.218675
(Hartree/Particle)
Thermal correction to Energy= 0.236432
Thermal correction to Enthalpy= 0.237376
Thermal correction to Gibbs Free Energy= 0.164759
Sum of electronic and zero-point Energies= -1176.536592
Sum of electronic and thermal Energies= -1176.518835
Sum of electronic and thermal Enthalpies= -1176.517891
Sum of electronic and thermal Free Energies= -1176.590508

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.363	66.747	152.836

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.720697	-0.229601	-1.047569
2	6	0	-1.537747	0.503432	-1.023396
3	6	0	-1.281335	1.428029	0.002430
4	6	0	-2.243498	1.592679	1.005478
5	6	0	-3.433954	0.860527	0.992648
6	6	0	-3.674272	-0.051161	-0.036363
7	1	0	-2.906050	-0.936655	-1.850782

8	1	0	-0.802131	0.354204	-1.809983
9	1	0	-2.067773	2.305617	1.807778
10	1	0	-4.168959	1.004065	1.777837
11	6	0	0.001070	2.245208	0.009051
12	1	0	0.008247	2.912526	-0.862555
13	1	0	-0.000946	2.897635	0.891814
14	6	0	1.276595	1.417779	0.001926
15	6	0	2.228457	1.572203	-1.012561
16	6	0	1.534411	0.489109	1.023655
17	6	0	3.410764	0.826947	-1.014046
18	1	0	2.049609	2.285106	-1.814205
19	6	0	2.708788	-0.258025	1.032888
20	1	0	0.804661	0.344780	1.816637
21	6	0	3.651153	-0.091137	0.009343
22	1	0	4.135563	0.958815	-1.810722
23	1	0	2.892149	-0.973195	1.829297
24	6	0	4.933755	-0.876507	0.054397
25	6	0	-4.929898	-0.879958	-0.055810
26	9	0	-4.695972	-2.164949	0.331094
27	9	0	-5.473865	-0.951850	-1.298802
28	9	0	-5.888223	-0.394572	0.770012
29	9	0	5.582720	-0.883525	-1.135162
30	9	0	4.726455	-2.172836	0.403305
31	9	0	5.806005	-0.371162	0.970935

1b+_tropylium_1.log

SCF Done: E(RB3LYP) = -1175.85011399 A.U. after 1 cycles

Zero-point correction= 0.208746
(Hartree/Particle)
Thermal correction to Energy= 0.226099
Thermal correction to Enthalpy= 0.227043
Thermal correction to Gibbs Free Energy= 0.159315
Sum of electronic and zero-point Energies= -1175.641368
Sum of electronic and thermal Energies= -1175.624015
Sum of electronic and thermal Enthalpies= -1175.623071
Sum of electronic and thermal Free Energies= -1175.690799

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	141.879	65.697	142.547

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

1	6	0	-2.674260	-0.896162	0.172307
2	6	0	-3.693606	0.061111	-0.008479
3	6	0	-3.537472	1.414472	-0.268455
4	6	0	-1.294091	-0.746477	0.144298
5	6	0	-2.333282	2.130878	-0.409377
6	6	0	-0.493825	0.401087	-0.085037
7	6	0	-1.016591	1.696119	-0.335469
8	1	0	-3.017825	-1.907121	0.379929
9	1	0	-4.447611	1.996289	-0.381096
10	1	0	-0.743028	-1.657779	0.358056
11	1	0	-2.456780	3.189930	-0.624606
12	1	0	-0.274475	2.466482	-0.524941
13	6	0	0.971825	0.238119	-0.061555
14	6	0	1.800130	1.248363	0.473507
15	6	0	1.574358	-0.930428	-0.575303
16	6	0	3.180926	1.088230	0.507271
17	1	0	1.367601	2.142324	0.912948
18	6	0	2.957228	-1.077675	-0.565582
19	1	0	0.970200	-1.706895	-1.035164
20	6	0	3.761118	-0.071562	-0.018679
21	1	0	3.805569	1.862243	0.940779
22	1	0	3.410363	-1.966620	-0.991518
23	6	0	5.264441	-0.258053	0.049833
24	6	0	-5.117888	-0.497186	0.108767
25	9	0	-6.052952	0.445424	-0.078394
26	9	0	-5.297623	-1.037254	1.330613
27	9	0	-5.304822	-1.468372	-0.807263
28	9	0	5.616567	-0.840638	1.219852
29	9	0	5.913578	0.922091	-0.027782
30	9	0	5.713244	-1.046124	-0.948435

1b+_tropylium_2.log

SCF Done: E(RB3LYP) = -1175.85016099 A.U. after 12 cycles

Zero-point correction= 0.208745
(Hartree/Particle)
Thermal correction to Energy= 0.226102
Thermal correction to Enthalpy= 0.227047
Thermal correction to Gibbs Free Energy= 0.159053
Sum of electronic and zero-point Energies= -1175.641416
Sum of electronic and thermal Energies= -1175.624059
Sum of electronic and thermal Enthalpies= -1175.623114
Sum of electronic and thermal Free Energies= -1175.691108

E (Thermal) CV S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	141.881	65.691	143.104

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.322244	2.124131	0.421046
2	6	0	3.530789	1.414261	0.284424
3	6	0	3.695258	0.063990	0.013612
4	6	0	1.008249	1.684283	0.331082
5	6	0	2.681844	-0.895966	-0.185092
6	6	0	0.493476	0.389295	0.064391
7	6	0	1.300803	-0.752622	-0.168273
8	1	0	2.439071	3.181680	0.647112
9	1	0	0.260908	2.449547	0.520901
10	1	0	3.031728	-1.903504	-0.398783
11	1	0	0.755774	-1.664327	-0.395321
12	6	0	-0.971279	0.220720	0.028025
13	6	0	-1.573060	-0.954891	0.526228
14	6	0	-1.799244	1.231537	-0.506482
15	6	0	-2.955168	-1.107621	0.504115
16	1	0	-0.969090	-1.734590	0.980831
17	6	0	-3.179050	1.066030	-0.552978
18	1	0	-1.366377	2.128836	-0.938801
19	6	0	-3.758643	-0.100723	-0.041922
20	1	0	-3.407349	-2.006528	0.909743
21	1	0	-3.802481	1.836384	-0.994633
22	6	0	-5.267558	-0.251059	-0.035675
23	9	0	-5.791853	0.280824	1.093362
24	9	0	-5.637830	-1.547034	-0.084824
25	9	0	-5.832519	0.383137	-1.083794
26	1	0	4.437299	1.998962	0.410654
27	6	0	5.123033	-0.486970	-0.095573
28	9	0	6.052142	0.458359	0.106866
29	9	0	5.306486	-1.464291	0.814607
30	9	0	5.315836	-1.016864	-1.319914

1b_carbene_s.log

SCF Done: E(RB3LYP) = -1175.43294089 A.U. after 1 cycles

Zero-point correction= 0.193382
(Hartree/Particle)
Thermal correction to Energy= 0.210864
Thermal correction to Enthalpy= 0.211808

Thermal correction to Gibbs Free Energy= 0.141659
Sum of electronic and zero-point Energies= -1175.239559
Sum of electronic and thermal Energies= -1175.222077
Sum of electronic and thermal Enthalpies= -1175.221133
Sum of electronic and thermal Free Energies= -1175.291282

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	132.319	65.815	147.640

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.707460	-0.620436	-0.738437
2	6	0	-1.451356	-0.022940	-0.700800
3	6	0	-1.239276	1.191847	0.009136
4	6	0	-2.350313	1.766943	0.685437
5	6	0	-3.580888	1.127857	0.713983
6	6	0	-3.765086	-0.060406	-0.012201
7	1	0	-2.861441	-1.533095	-1.305063
8	1	0	-0.629226	-0.467277	-1.253504
9	1	0	-2.206507	2.715812	1.193156
10	1	0	-4.410360	1.560676	1.264862
11	6	0	-0.000001	1.909286	-0.000003
12	6	0	1.239277	1.191849	-0.009121
13	6	0	2.350304	1.766942	-0.685443
14	6	0	1.451367	-0.022928	0.700826
15	6	0	3.580879	1.127856	-0.714005
16	1	0	2.206486	2.715808	-1.193164
17	6	0	2.707471	-0.620423	0.738447
18	1	0	0.629246	-0.467259	1.253549
19	6	0	3.765085	-0.060402	0.012185
20	1	0	4.410343	1.560668	-1.264900
21	1	0	2.861463	-1.533075	1.305082
22	6	0	5.133956	-0.690895	0.048665
23	6	0	-5.133957	-0.690895	-0.048670
24	9	0	-5.732547	-0.669334	1.168737
25	9	0	-5.099787	-1.982009	-0.454746
26	9	0	-5.966475	-0.032644	-0.899765
27	9	0	5.732648	-0.669143	-1.168691
28	9	0	5.099753	-1.982070	0.454535
29	9	0	5.966406	-0.032777	0.899930

b_carbene_t.log

SCF Done: E(UB3LYP) = -1175.44405578 A.U. after 12 cycles

Zero-point correction=	0.192626
(Hartree/Particle)	
Thermal correction to Energy=	0.210288
Thermal correction to Enthalpy=	0.211232
Thermal correction to Gibbs Free Energy=	0.139738
Sum of electronic and zero-point Energies=	-1175.251430
Sum of electronic and thermal Energies=	-1175.233768
Sum of electronic and thermal Enthalpies=	-1175.232824
Sum of electronic and thermal Free Energies=	-1175.304317

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	131.958	66.215	150.471

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.682715	1.214770	-0.559908
2	6	0	-2.360158	1.629797	-0.582932
3	6	0	-1.330926	0.833078	-0.001382
4	6	0	-1.713393	-0.395078	0.620912
5	6	0	-3.038884	-0.801886	0.635494
6	6	0	-4.031694	-0.001926	0.047786
7	1	0	-4.451385	1.835054	-1.009991
8	1	0	-2.092759	2.572910	-1.049695
9	1	0	-0.953406	-1.008134	1.095866
10	1	0	-3.310522	-1.737795	1.113952
11	6	0	0.000989	1.267797	0.000144
12	6	0	1.329661	0.823602	0.018614
13	6	0	1.702460	-0.431713	-0.553303
14	6	0	2.364469	1.633184	0.571704
15	6	0	3.024277	-0.850375	-0.548308
16	1	0	0.937421	-1.058505	-1.001474
17	6	0	3.683417	1.206033	0.568397
18	1	0	2.103724	2.594052	1.004813
19	6	0	4.022175	-0.038824	0.014493
20	1	0	3.287519	-1.810399	-0.981642
21	1	0	4.455449	1.833252	1.002800
22	6	0	5.459910	-0.475536	-0.034108
23	6	0	-5.458597	-0.474447	0.020790
24	9	0	-5.725067	-1.221171	-1.088298
25	9	0	-6.341877	0.554643	0.010476
26	9	0	-5.763412	-1.253521	1.088526
27	9	0	5.589133	-1.825153	0.015060
28	9	0	6.187699	0.033993	0.990632
29	9	0	6.075525	-0.072268	-1.181395

1c+_a.log

```
 SCF Done:  E(RB3LYP) =  -799.465906986     A.U. after    1 cycles


 Zero-point correction=                           0.174378
(Hartree/Particle)
 Thermal correction to Energy=                    0.186918
 Thermal correction to Enthalpy=                  0.187862
 Thermal correction to Gibbs Free Energy=         0.134212
 Sum of electronic and zero-point Energies=           -799.291529
 Sum of electronic and thermal Energies=              -799.278989
 Sum of electronic and thermal Enthalpies=            -799.278045
 Sum of electronic and thermal Free Energies=         -799.331695

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 117.293             49.197           112.917
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.934365	-0.414011	0.183749
2	6	0	-2.701114	-1.026417	0.275280
3	6	0	-1.532301	-0.291947	-0.090448
4	6	0	-1.679260	1.028542	-0.614103
5	6	0	-2.938106	1.598727	-0.717786
6	6	0	-4.076447	0.889257	-0.304632
7	1	0	-2.631440	-2.042525	0.651482
8	1	0	-0.818197	1.562204	-0.997194
9	6	0	-0.291666	-0.959093	0.055429
10	1	0	-0.369886	-2.039253	0.179005
11	6	0	1.042796	-0.463997	0.068484
12	6	0	1.381689	0.896847	0.308850
13	6	0	2.077707	-1.420174	-0.140146
14	6	0	2.715796	1.258170	0.291808
15	1	0	0.639272	1.637873	0.575613
16	6	0	3.393082	-0.990192	-0.174054
17	1	0	1.852009	-2.469369	-0.301136
18	6	0	3.743860	0.343082	0.041806
19	1	0	-5.069704	1.322585	-0.377680
20	9	0	3.048452	2.530806	0.539482
21	9	0	4.366433	-1.878923	-0.399420
22	1	0	4.783126	0.656678	0.040811
23	9	0	-5.030712	-1.086861	0.555404
24	1	0	-3.052758	2.593845	-1.135505

1c+_b.log

```
SCF Done:  E(RB3LYP) =  -799.466496297     A.U. after    1 cyc

 Zero-point correction=                           0.174424
(Hartree/Particle)
 Thermal correction to Energy=                    0.186956
 Thermal correction to Enthalpy=                  0.187900
 Thermal correction to Gibbs Free Energy=         0.134243
 Sum of electronic and zero-point Energies=           -799.292073
 Sum of electronic and thermal Energies=              -799.279541
 Sum of electronic and thermal Enthalpies=            -799.278596
 Sum of electronic and thermal Free Energies=         -799.332253

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 117.316             49.178           112.930

-------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000007316    0.000001638    0.000000369
      2        6          -0.000005447   -0.000004204   -0.000006512
      3        6          -0.000003099   -0.000029785   -0.000011839
      4        6           0.000007471    0.000021240    0.000011532
      5        6          -0.000008397    0.000006515   -0.000002423
      6        6          -0.000010181   -0.000021779   -0.000004357
      7        1           0.000001667    0.000004343    0.000000526
      8        1           0.000002601   -0.000001546    0.000002184
      9        6          -0.000009936   -0.000000466   -0.000000237
     10        1           0.000002860    0.000001784    0.000002940
     11        6           0.000004156    0.000006336   -0.000009864
     12        6          -0.000003570    0.000024608   -0.000004821
     13        6           0.000008111   -0.000036427    0.000014839
     14        6          -0.000006868   -0.000000212   -0.000002223
     15        1           0.000000568   -0.000004216    0.000001499
     16        6           0.000017660   -0.000012912    0.000009994
     17        1          -0.000001174    0.000007234   -0.000001645
     18        6          -0.000016550    0.000010892   -0.000005639
     19        9           0.000012261   -0.000008109    0.000003498
     20        9          -0.000004096    0.000021878   -0.000009350
     21        1          -0.000006513   -0.000008419    0.000002674
     22        1           0.000012377   -0.000002725   -0.000000820
     23        9           0.000000888    0.000014069    0.000005762
     24        1           0.000012528    0.000010263    0.000003913
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```

1cH.log

SCF Done: E(RB3LYP) = -800.359702022 A.U. after 1 cycles

Zero-point correction= 0.185097
(Hartree/Particle)
Thermal correction to Energy= 0.197965
Thermal correction to Enthalpy= 0.198909
Thermal correction to Gibbs Free Energy= 0.142506
Sum of electronic and zero-point Energies= -800.174605
Sum of electronic and thermal Energies= -800.161737
Sum of electronic and thermal Enthalpies= -800.160793
Sum of electronic and thermal Free Energies= -800.217196

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	124.225	50.183	118.711

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.093331	0.662942	0.832598
2	6	0	1.894847	0.893771	0.173407
3	6	0	1.553106	0.088891	-0.924450
4	6	0	2.434837	-0.925584	-1.319768
5	6	0	3.637013	-1.137156	-0.635303
6	6	0	3.981680	-0.339158	0.456521
7	1	0	1.239908	1.688407	0.519494
8	1	0	2.183833	-1.553105	-2.171574
9	6	0	0.251130	0.329361	-1.671101
10	1	0	0.238680	1.353777	-2.063405
11	1	0	0.218689	-0.333305	-2.545613
12	6	0	-1.005164	0.111823	-0.839712
13	6	0	-1.986338	1.109083	-0.768821
14	6	0	-1.205173	-1.098311	-0.157371
15	6	0	-3.138948	0.874537	-0.025553
16	1	0	-1.868442	2.058109	-1.282624
17	6	0	-2.374949	-1.277323	0.567242
18	1	0	-0.462939	-1.889944	-0.178433
19	6	0	-3.371227	-0.310192	0.659268
20	1	0	4.906911	-0.479587	1.005959
21	9	0	-4.081430	1.849530	0.035951
22	9	0	-2.563151	-2.451466	1.221883
23	1	0	-4.275054	-0.472314	1.234888
24	9	0	3.413889	1.453081	1.892661
25	1	0	4.309757	-1.928454	-0.954887

1c+_a_tropylium_1.log

SCF Done: E(RB3LYP) = -799.467479338 A.U. after 1 cycles

Zero-point correction= 0.175090
(Hartree/Particle)
Thermal correction to Energy= 0.187506
Thermal correction to Enthalpy= 0.188450
Thermal correction to Gibbs Free Energy= 0.135442
Sum of electronic and zero-point Energies= -799.292389
Sum of electronic and thermal Energies= -799.279973
Sum of electronic and thermal Enthalpies= -799.279029
Sum of electronic and thermal Free Energies= -799.332037

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.662	48.848	111.566

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.337759	1.291121	-0.304676
2	6	0	-3.372371	0.361615	-0.156867
3	6	0	-3.200960	-0.976330	0.138459
4	6	0	-0.951628	1.166177	-0.216790
5	6	0	-2.017285	-1.714338	0.357524
6	6	0	-0.177869	0.032168	0.076780
7	6	0	-0.713498	-1.269171	0.332682
8	1	0	-0.420771	2.088157	-0.435369
9	1	0	-2.182591	-2.764064	0.588637
10	1	0	0.024349	-2.028713	0.572553
11	6	0	1.288267	0.191149	0.129653
12	6	0	2.132274	-0.844332	-0.324646
13	6	0	1.864752	1.376120	0.635934
14	6	0	3.505654	-0.659929	-0.276237
15	1	0	1.748748	-1.759388	-0.764137
16	6	0	3.250193	1.517194	0.693182
17	1	0	1.237040	2.166496	1.035845
18	6	0	4.088509	0.500595	0.228639
19	1	0	3.682916	2.422505	1.107264
20	1	0	-4.388314	0.724454	-0.289731
21	1	0	5.169540	0.593345	0.253094
22	9	0	4.299894	-1.640518	-0.740920
23	9	0	-4.320996	-1.690046	0.239666
24	9	0	-2.758964	2.522229	-0.604299

1c+_b_tropylium_1.log

SCF Done: E(RB3LYP) = -799.467441925 A.U. after 1 cycles

Zero-point correction= (Hartree/Particle)	0.175098
Thermal correction to Energy=	0.187512
Thermal correction to Enthalpy=	0.188456
Thermal correction to Gibbs Free Energy=	0.135452
Sum of electronic and zero-point Energies=	-799.292344
Sum of electronic and thermal Energies=	-799.279930
Sum of electronic and thermal Enthalpies=	-799.278986
Sum of electronic and thermal Free Energies=	-799.331990

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.666	48.843	111.556

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.092344	1.410975	-0.290195
2	6	0	-3.273923	0.695577	-0.069977
3	6	0	-3.342611	-0.652692	0.219811
4	6	0	-0.752969	1.022543	-0.291308
5	6	0	-2.310301	-1.605212	0.364110
6	6	0	-0.192875	-0.240987	-0.044471
7	6	0	-0.949819	-1.417717	0.252103
8	1	0	-0.071071	1.828712	-0.546177
9	1	0	-2.658195	-2.605462	0.611273
10	1	0	-0.356772	-2.305678	0.448123
11	6	0	1.276714	-0.368124	-0.087971
12	6	0	1.884255	-1.537208	-0.595293
13	6	0	2.093108	0.689176	0.366096
14	6	0	3.273159	-1.638292	-0.659759
15	1	0	1.279823	-2.346818	-0.992499
16	6	0	3.470740	0.544306	0.311139
17	1	0	1.683224	1.591621	0.807906
18	6	0	4.084117	-0.598967	-0.197885
19	1	0	-4.208034	1.247309	-0.136776
20	1	0	5.167224	-0.662384	-0.224172
21	9	0	-4.569414	-1.139928	0.398286
22	9	0	-2.288662	2.701914	-0.567892
23	9	0	4.239266	1.545081	0.775082

24	1	0	3.729572	-2.531174	-1.075375

1c+_a_tropylium_2.log

SCF Done: E(RB3LYP) = -799.466680405 A.U. after 1 cycles

Zero-point correction= 0.175195
(Hartree/Particle)
Thermal correction to Energy= 0.187647
Thermal correction to Enthalpy= 0.188591
Thermal correction to Gibbs Free Energy= 0.135484
Sum of electronic and zero-point Energies= -799.291486
Sum of electronic and thermal Energies= -799.279033
Sum of electronic and thermal Enthalpies= -799.278089
Sum of electronic and thermal Free Energies= -799.331197

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.750	48.948	111.775

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.556430	-1.648455	-0.733656
2	6	0	3.716393	-0.941901	-0.405505
3	6	0	3.774891	0.323835	0.164631
4	6	0	1.212603	-1.293792	-0.589378
5	6	0	2.733455	1.186006	0.547117
6	6	0	0.631137	-0.124623	-0.056665
7	6	0	1.368346	0.980420	0.451909
8	1	0	0.510207	-2.030168	-0.969302
9	1	0	0.766325	1.790365	0.853707
10	6	0	-0.845712	-0.035938	-0.020136
11	6	0	-1.489007	1.190414	-0.280488
12	6	0	-1.615624	-1.179124	0.272260
13	6	0	-2.877458	1.237190	-0.255600
14	1	0	-0.944668	2.087563	-0.554955
15	6	0	-2.999798	-1.063980	0.306348
16	1	0	-1.166745	-2.133364	0.525724
17	6	0	-3.665415	0.129119	0.041006
18	1	0	-4.747848	0.192692	0.065333
19	1	0	2.727912	-2.622869	-1.185225
20	1	0	3.064355	2.124685	0.985823
21	1	0	4.675291	-1.410190	-0.613372
22	9	0	-3.725594	-2.150719	0.613346

23	9	0	-3.484052	2.402158	-0.533021
24	9	0	5.000060	0.798146	0.390919

1c+_b_tropylium_2.log

SCF Done: E(RB3LYP) = -799.466932000 A.U. after 1 cycles

Zero-point correction= 0.175156
(Hartree/Particle)
Thermal correction to Energy= 0.187621
Thermal correction to Enthalpy= 0.188565
Thermal correction to Gibbs Free Energy= 0.135481
Sum of electronic and zero-point Energies= -799.291776
Sum of electronic and thermal Energies= -799.279311
Sum of electronic and thermal Enthalpies= -799.278367
Sum of electronic and thermal Free Energies= -799.331451

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.734	48.962	111.726

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.917023	0.957944	0.365934
2	6	0	3.947940	0.055819	0.052962
3	6	0	3.792970	-1.237928	-0.409194
4	6	0	1.532865	0.830604	0.318274
5	6	0	2.593022	-1.935365	-0.667204
6	6	0	0.754553	-0.269639	-0.086628
7	6	0	1.279106	-1.515098	-0.531339
8	1	0	1.002260	1.710697	0.671001
9	1	0	0.533364	-2.243561	-0.836097
10	6	0	-0.717077	-0.116656	-0.049012
11	6	0	-1.531210	-1.201161	0.333559
12	6	0	-1.309796	1.114359	-0.393111
13	6	0	-2.908451	-1.022158	0.375186
14	1	0	-1.121990	-2.154162	0.650630
15	6	0	-2.694323	1.224326	-0.356303
16	1	0	-0.729999	1.963525	-0.738400
17	6	0	-3.525140	0.176641	0.030001
18	1	0	-4.603477	0.289096	0.059657
19	1	0	2.719614	-2.948724	-1.041135
20	1	0	4.955492	0.436794	0.200554
21	9	0	-3.254051	2.390739	-0.713035

22	9	0	-3.676128	-2.050626	0.768515
23	1	0	4.711162	-1.787305	-0.601911
24	9	0	3.346255	2.144721	0.804183

1c_carbene_s.log

SCF Done: E(RB3LYP) = -799.038173565 A.U. after 1 cycles

Zero-point correction= 0.159779
(Hartree/Particle)
Thermal correction to Energy= 0.172381
Thermal correction to Enthalpy= 0.173326
Thermal correction to Gibbs Free Energy= 0.119439
Sum of electronic and zero-point Energies= -798.878395
Sum of electronic and thermal Energies= -798.865792
Sum of electronic and thermal Enthalpies= -798.864848
Sum of electronic and thermal Free Energies= -798.918735

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	108.171	49.228	113.414

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.066520	0.693809	-0.714638
2	6	0	-1.773196	0.217749	-0.600213
3	6	0	-1.519015	-0.898698	0.247895
4	6	0	-2.612695	-1.469310	0.955107
5	6	0	-3.885076	-0.913408	0.875021
6	6	0	-4.129321	0.167163	0.017077
7	1	0	-0.978021	0.672748	-1.181042
8	1	0	-2.419970	-2.344541	1.567320
9	6	0	-0.237513	-1.526930	0.377367
10	6	0	0.956641	-0.744690	0.227424
11	6	0	1.090058	0.576791	0.738725
12	6	0	2.086041	-1.360721	-0.375558
13	6	0	2.318416	1.211091	0.648840
14	1	0	0.261680	1.074988	1.229692
15	6	0	3.256637	-0.637601	-0.509552
16	1	0	2.021790	-2.384542	-0.726475
17	6	0	3.419807	0.646086	0.012161
18	1	0	-5.123243	0.586613	-0.104772
19	9	0	2.455720	2.455279	1.172773
20	9	0	4.320786	-1.210048	-1.124703

21	1	0	4.365837	1.170766	-0.058242
22	9	0	-3.315098	1.732084	-1.555664
23	1	0	-4.706324	-1.339876	1.443934

1c_carbene_t.log

SCF Done: E(UB3LYP) = -799.047350544 A.U. after 1 cycles

Zero-point correction= 0.158994
(Hartree/Particle)
Thermal correction to Energy= 0.171768
Thermal correction to Enthalpy= 0.172712
Thermal correction to Gibbs Free Energy= 0.116836
Sum of electronic and zero-point Energies= -798.888357
Sum of electronic and thermal Energies= -798.875583
Sum of electronic and thermal Enthalpies= -798.874638
Sum of electronic and thermal Free Energies= -798.930515

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	107.786	49.670	117.602

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.423718	0.693195	0.523622
2	6	0	-2.072089	0.406562	0.529962
3	6	0	-1.606161	-0.744599	-0.174232
4	6	0	-2.566618	-1.561718	-0.838706
5	6	0	-3.916695	-1.234050	-0.812640
6	6	0	-4.369036	-0.095746	-0.130612
7	1	0	-1.385256	1.046865	1.073127
8	1	0	-2.224047	-2.444344	-1.369754
9	6	0	-0.245712	-1.090968	-0.176175
10	6	0	1.045050	-0.545845	-0.104067
11	6	0	1.305388	0.789843	-0.538293
12	6	0	2.134773	-1.333832	0.367257
13	6	0	2.597680	1.275426	-0.470348
14	1	0	0.510704	1.416591	-0.926957
15	6	0	3.399948	-0.779124	0.400020
16	1	0	1.976571	-2.353335	0.700269
17	6	0	3.678700	0.525441	-0.007605
18	1	0	-5.418418	0.177754	-0.098149
19	9	0	2.838123	2.546270	-0.880958
20	9	0	4.431194	-1.534192	0.855061

21	1	0	4.681828	0.933364	0.029853
22	9	0	-3.855570	1.794751	1.193838
23	1	0	-4.634161	-1.865860	-1.328953

1d+.log

SCF Done: E(RB3LYP) = -700.233717288 A.U. after 2 cycles

Zero-point correction= 0.182871
(Hartree/Particle)
Thermal correction to Energy= 0.194540
Thermal correction to Enthalpy= 0.195484
Thermal correction to Gibbs Free Energy= 0.143902
Sum of electronic and zero-point Energies= -700.050847
Sum of electronic and thermal Energies= -700.039177
Sum of electronic and thermal Enthalpies= -700.038233
Sum of electronic and thermal Free Energies= -700.089815

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	122.076	46.185	108.563

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.674507	1.188208	0.449661
2	6	0	2.378938	1.679450	0.363064
3	6	0	1.294927	0.818496	0.014123
4	6	0	1.570726	-0.539778	-0.316379
5	6	0	2.873807	-0.984741	-0.244583
6	6	0	3.933161	-0.152359	0.143632
7	1	0	2.177476	2.722491	0.589187
8	1	0	0.805888	-1.211886	-0.684465
9	6	0	0.000000	1.398962	0.000003
10	6	0	-1.294927	0.818496	-0.014120
11	6	0	-1.570726	-0.539778	0.316380
12	6	0	-2.378937	1.679450	-0.363064
13	6	0	-2.873807	-0.984741	0.244582
14	1	0	-0.805889	-1.211886	0.684467
15	6	0	-3.674506	1.188209	-0.449663
16	1	0	-2.177474	2.722491	-0.589188
17	6	0	-3.933161	-0.152358	-0.143634
18	1	0	0.000000	2.488831	-0.000000
19	1	0	4.939904	-0.558414	0.176276
20	1	0	-4.939904	-0.558413	-0.176279

21	1	0	4.490987	1.842579	0.737159
22	9	0	3.148178	-2.254637	-0.575606
23	1	0	-4.490986	1.842579	-0.737162
24	9	0	-3.148180	-2.254636	0.575606

1dH.log

SCF Done: E(RB3LYP) = -701.118682771 A.U. after 1 cycles

Zero-point correction= 0.193391
(Hartree/Particle)
Thermal correction to Energy= 0.205411
Thermal correction to Enthalpy= 0.206355
Thermal correction to Gibbs Free Energy= 0.151982
Sum of electronic and zero-point Energies= -700.925292
Sum of electronic and thermal Energies= -700.913271
Sum of electronic and thermal Enthalpies= -700.912327
Sum of electronic and thermal Free Energies= -700.966701

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	128.898	47.176	114.439

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.799104	1.105371	0.191673
2	6	0	1.568891	0.722101	-0.322107
3	6	0	1.343874	-0.631047	-0.619142
4	6	0	2.371285	-1.553986	-0.381725
5	6	0	3.602247	-1.139548	0.138624
6	6	0	3.831578	0.205433	0.433237
7	6	0	0.015726	-1.077524	-1.212895
8	1	0	-0.083887	-0.663722	-2.224879
9	1	0	0.034708	-2.168430	-1.330686
10	6	0	-1.206459	-0.682629	-0.399038
11	6	0	-2.187844	0.150245	-0.950534
12	6	0	-1.378205	-1.153908	0.912612
13	6	0	-3.302077	0.485562	-0.188010
14	6	0	-2.506664	-0.802727	1.654578
15	6	0	-3.490464	0.029214	1.108356
16	9	0	3.003885	2.421399	0.472550
17	9	0	-4.244723	1.295892	-0.742759
18	1	0	-4.376401	0.317924	1.664667
19	1	0	-2.626009	-1.176438	2.668072

20	1	0	-0.619715	-1.794731	1.355294
21	1	0	-2.100084	0.536292	-1.962235
22	1	0	0.799386	1.472406	-0.479153
23	1	0	4.775248	0.556085	0.838500
24	1	0	4.387785	-1.869087	0.316909
25	1	0	2.210556	-2.605257	-0.608391

1dH_tropylium_1.log

SCF Done: E(RB3LYP) = -700.231557667 A.U. after 2 cycles

Zero-point correction= 0.183556
(Hartree/Particle)
Thermal correction to Energy= 0.195152
Thermal correction to Enthalpy= 0.196096
Thermal correction to Gibbs Free Energy= 0.145120
Sum of electronic and zero-point Energies= -700.048002
Sum of electronic and thermal Energies= -700.036405
Sum of electronic and thermal Enthalpies= -700.035461
Sum of electronic and thermal Free Energies= -700.086438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	122.460	45.986	107.289

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.537696	1.121856	0.242971
2	6	0	-1.177641	0.838321	0.260658
3	6	0	-1.169648	-1.591930	-0.357589
4	6	0	-2.518012	-1.874081	-0.504247
5	6	0	-3.638104	-1.025839	-0.359392
6	6	0	-3.657044	0.314602	-0.025474
7	1	0	-0.561320	1.684277	0.551821
8	1	0	-2.749405	-2.898063	-0.788270
9	6	0	-0.515805	-0.375448	-0.010405
10	6	0	0.958837	-0.384638	0.068019
11	6	0	1.646212	-1.512705	0.565111
12	6	0	1.697909	0.743657	-0.344865
13	6	0	3.037207	-1.505666	0.658122
14	1	0	1.098597	-2.375526	0.931286
15	6	0	3.081461	0.706357	-0.262743
16	1	0	1.226794	1.621341	-0.775538
17	6	0	3.772862	-0.395838	0.235812

18	1	0	-0.504498	-2.424454	-0.566885
19	1	0	-4.617718	0.818374	0.046587
20	1	0	4.856766	-0.374149	0.285607
21	9	0	3.777667	1.775304	-0.688864
22	1	0	3.554220	-2.368780	1.065646
23	9	0	-2.842079	2.385928	0.554517
24	1	0	-4.606953	-1.485991	-0.536995

1dH_tropylium_2.log

SCF Done: E(RB3LYP) = -700.231630453 A.U. after 1 cycles

Zero-point correction= 0.183567
(Hartree/Particle)
Thermal correction to Energy= 0.195159
Thermal correction to Enthalpy= 0.196103
Thermal correction to Gibbs Free Energy= 0.145154
Sum of electronic and zero-point Energies= -700.048064
Sum of electronic and thermal Energies= -700.036472
Sum of electronic and thermal Enthalpies= -700.035528
Sum of electronic and thermal Free Energies= -700.086476

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	122.464	45.979	107.230

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.772262	-0.874357	0.279840
2	6	0	1.384986	-0.892862	0.206203
3	6	0	0.889660	1.488679	-0.402012
4	6	0	2.150818	2.059754	-0.453239
5	6	0	3.416540	1.472437	-0.234054
6	6	0	3.704410	0.161621	0.094132
7	1	0	0.949373	-1.856961	0.452590
8	1	0	2.171787	3.114963	-0.715630
9	6	0	0.494347	0.153016	-0.106073
10	6	0	-0.948183	-0.161954	-0.131468
11	6	0	-1.890871	0.790091	0.310136
12	6	0	-1.402966	-1.412162	-0.602857
13	6	0	-3.238003	0.463039	0.281966
14	1	0	-1.599586	1.750346	0.723033
15	6	0	-2.766789	-1.697749	-0.640780
16	1	0	-0.700163	-2.143175	-0.990772

17	6	0	-3.701921	-0.763100	-0.189549
18	1	0	0.075114	2.161538	-0.653255
19	1	0	4.744642	-0.123004	0.231338
20	1	0	-4.767550	-0.968395	-0.198380
21	9	0	3.323187	-2.048835	0.604563
22	1	0	4.271489	2.135462	-0.340785
23	1	0	-3.106681	-2.652977	-1.028535
24	9	0	-4.125872	1.367001	0.733985

1d_carbene_s.log

SCF Done: E(RB3LYP) = -699.798303207 A.U. after 1 cycles

Zero-point correction= 0.168151
(Hartree/Particle)
Thermal correction to Energy= 0.179878
Thermal correction to Enthalpy= 0.180822
Thermal correction to Gibbs Free Energy= 0.129095
Sum of electronic and zero-point Energies= -699.630152
Sum of electronic and thermal Energies= -699.618425
Sum of electronic and thermal Enthalpies= -699.617481
Sum of electronic and thermal Free Energies= -699.669208

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.875	46.203	108.869

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929283	0.879279	-0.414615
2	6	0	1.607368	0.471658	-0.435763
3	6	0	1.284277	-0.853197	-0.024556
4	6	0	2.342782	-1.698653	0.406836
5	6	0	3.647920	-1.225723	0.491178
6	6	0	3.960008	0.070008	0.057156
7	6	0	-0.037077	-1.407318	-0.096284
8	6	0	-1.172175	-0.559561	0.129636
9	6	0	-2.376814	-0.866574	-0.560318
10	6	0	-1.191867	0.506078	1.074525
11	6	0	-3.494495	-0.082265	-0.351498
12	6	0	-2.362351	1.221450	1.317354
13	6	0	-3.524301	0.950016	0.586499
14	1	0	-2.405458	-1.705431	-1.247543
15	1	0	-4.441762	1.509274	0.741111

16	1	0	-0.293060	0.729852	1.640228
17	1	0	0.840708	1.147702	-0.799049
18	1	0	4.978896	0.444678	0.060029
19	1	0	2.098731	-2.720872	0.678275
20	9	0	3.238655	2.131392	-0.848065
21	9	0	-4.630021	-0.350886	-1.048458
22	1	0	4.442052	-1.873306	0.852184
23	1	0	-2.373158	2.012362	2.062577

1d_carbene_t.log

SCF Done: E(UB3LYP) = -699.807177757 A.U. after 1 cycles

Zero-point correction= 0.167290
(Hartree/Particle)
Thermal correction to Energy= 0.179212
Thermal correction to Enthalpy= 0.180156
Thermal correction to Gibbs Free Energy= 0.126384
Sum of electronic and zero-point Energies= -699.639888
Sum of electronic and thermal Energies= -699.627966
Sum of electronic and thermal Enthalpies= -699.627022
Sum of electronic and thermal Free Energies= -699.680794

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	112.457	46.674	113.173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.244112	0.754641	-0.379626
2	6	0	1.876144	0.562052	-0.384158
3	6	0	1.349798	-0.680073	0.084932
4	6	0	2.271073	-1.677599	0.520135
5	6	0	3.639570	-1.438271	0.500720
6	6	0	4.151313	-0.212421	0.051566
7	6	0	-0.030697	-0.931224	0.077519
8	6	0	-1.280683	-0.297701	0.155875
9	6	0	-2.430314	-0.889104	-0.442947
10	6	0	-1.449990	0.928429	0.870581
11	6	0	-3.651919	-0.255643	-0.324193
12	6	0	-2.699648	1.530241	0.957821
13	6	0	-3.825714	0.946842	0.360199
14	1	0	-2.350690	-1.822713	-0.989467
15	1	0	-4.809991	1.399030	0.421185

16	1	0	-0.589920	1.381567	1.353622
17	1	0	1.219883	1.344439	-0.750093
18	1	0	5.216026	-0.005302	0.028915
19	1	0	1.883267	-2.629008	0.870732
20	9	0	3.732746	1.944462	-0.824296
21	9	0	-4.739777	-0.829347	-0.905490
22	1	0	4.325671	-2.209406	0.840262
23	1	0	-2.809241	2.464345	1.502368

1e+.log

```
 SCF Done:  E(RB3LYP) =  -997.910904594     A.U. after    1 cycles


 Zero-point correction=                           0.158379
(Hartree/Particle)
 Thermal correction to Energy=                    0.172910
 Thermal correction to Enthalpy=                  0.173855
 Thermal correction to Gibbs Free Energy=         0.115848
 Sum of electronic and zero-point Energies=           -997.752526
 Sum of electronic and thermal Energies=              -997.737994
 Sum of electronic and thermal Enthalpies=            -997.737050
 Sum of electronic and thermal Free Energies=         -997.795056

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 108.503             55.139            122.084


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.686946    0.973159    0.126815
      2          6           0        1.357415    1.348099    0.049516
      3          6           0        0.290936    0.403277   -0.080735
      4          6           0        0.683516   -0.962682   -0.184199
      5          6           0        2.010405   -1.352353   -0.131823
      6          6           0        3.014674   -0.386119    0.035520
      7          6           0       -1.025207    0.937003   -0.193378
      8          6           0       -2.321614    0.403002   -0.042873
      9          6           0       -2.649188   -0.848049    0.569829
     10          6           0       -3.394610    1.246936   -0.486036
     11          6           0       -3.970142   -1.233448    0.694158
     12          1           0       -1.871029   -1.481287    0.973019
     13          6           0       -4.710281    0.834686   -0.385009
     14          1           0       -3.160217    2.213734   -0.923372
     15          6           0       -4.998948   -0.406575    0.204432
```

16	1	0	-4.216770	-2.174414	1.175638
17	1	0	-1.018206	1.997819	-0.436616
18	9	0	3.645082	1.876895	0.281230
19	9	0	2.345153	-2.630360	-0.256909
20	1	0	-5.513632	1.470119	-0.743626
21	1	0	-6.032837	-0.727276	0.299874
22	9	0	1.066404	2.644222	0.136077
23	9	0	-0.222359	-1.911924	-0.413469
24	9	0	4.273417	-0.761090	0.097269

1eH.log

SCF Done: E(RB3LYP) = -998.808428594 A.U. after 1 cycles

Zero-point correction= 0.169183
(Hartree/Particle)
Thermal correction to Energy= 0.184013
Thermal correction to Enthalpy= 0.184957
Thermal correction to Gibbs Free Energy= 0.124906
Sum of electronic and zero-point Energies= -998.639246
Sum of electronic and thermal Energies= -998.624415
Sum of electronic and thermal Enthalpies= -998.623471
Sum of electronic and thermal Free Energies= -998.683523

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	115.470	56.084	126.389

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.164067	1.203823	0.153967
2	6	0	0.929691	1.185244	-0.490508
3	6	0	0.274716	-0.000037	-0.832523
4	6	0	0.929921	-1.185202	-0.490654
5	6	0	2.164322	-1.203622	0.153834
6	6	0	2.784249	0.000132	0.480368
7	6	0	-1.076659	-0.000109	-1.527340
8	1	0	-1.133155	0.880311	-2.174536
9	1	0	-1.133098	-0.880616	-2.174420
10	6	0	-2.253161	-0.000098	-0.557790
11	6	0	-2.802243	1.206509	-0.101473
12	6	0	-2.801558	-1.206737	-0.100699
13	6	0	-3.873245	1.207663	0.795969
14	1	0	-2.390407	2.150513	-0.450584

15	6	0	-3.872556	-1.207928	0.796739
16	1	0	-2.389195	-2.150730	-0.449215
17	6	0	-4.410948	-0.000138	1.249069
18	1	0	-4.288839	2.152453	1.137260
19	1	0	-4.287610	-2.152736	1.138636
20	1	0	-5.245645	-0.000152	1.945272
21	9	0	0.364045	-2.372328	-0.796450
22	9	0	2.758265	-2.366797	0.459391
23	9	0	3.970574	0.000252	1.101794
24	9	0	2.757827	2.367050	0.459677
25	9	0	0.363552	2.372264	-0.796209

1e_tropylium_1.log

SCF Done: E(RB3LYP) = -997.905275593 A.U. after 2 cycles

Zero-point correction= 0.158606
(Hartree/Particle)
Thermal correction to Energy= 0.172774
Thermal correction to Enthalpy= 0.173718
Thermal correction to Gibbs Free Energy= 0.116906
Sum of electronic and zero-point Energies= -997.746669
Sum of electronic and thermal Energies= -997.732502
Sum of electronic and thermal Enthalpies= -997.731558
Sum of electronic and thermal Free Energies= -997.788369

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	108.417	54.486	119.571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.516102	-1.424064	-0.122593
2	6	0	-0.148260	-1.141243	-0.110961
3	6	0	-0.128333	1.338601	0.105094
4	6	0	-1.473719	1.664417	0.127736
5	6	0	-2.612329	0.833433	0.086134
6	6	0	-2.620903	-0.551781	-0.023530
7	6	0	0.536733	0.097459	0.008146
8	6	0	2.010285	0.117084	0.007740
9	6	0	2.686088	1.133931	-0.706066
10	6	0	2.766697	-0.826911	0.738995
11	6	0	4.075171	1.194345	-0.698761
12	1	0	2.127903	1.845100	-1.309139

13	6	0	4.154646	-0.736936	0.766873
14	1	0	2.275627	-1.602002	1.316659
15	6	0	4.812460	0.264696	0.044148
16	1	0	0.513001	2.208824	0.213661
17	1	0	5.897075	0.319501	0.057351
18	9	0	-1.841180	-2.696861	-0.266741
19	1	0	4.725128	-1.450912	1.352947
20	1	0	4.583634	1.961499	-1.274651
21	9	0	-1.759663	2.956758	0.239340
22	9	0	-3.787013	1.427584	0.160457
23	9	0	-3.805394	-1.130945	-0.050914
24	9	0	0.595810	-2.229891	-0.270425

1e_tropylium_2.log

SCF Done: E(RB3LYP) = -997.908996514 A.U. after 2 cycles

Zero-point correction= 0.158894
(Hartree/Particle)
Thermal correction to Energy= 0.173439
Thermal correction to Enthalpy= 0.174383
Thermal correction to Gibbs Free Energy= 0.117004
Sum of electronic and zero-point Energies= -997.750102
Sum of electronic and thermal Energies= -997.735558
Sum of electronic and thermal Enthalpies= -997.734614
Sum of electronic and thermal Free Energies= -997.791993

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	108.834	55.218	120.764

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.400167	1.249543	-0.927676
2	6	0	2.038685	1.002812	-0.753950
3	6	0	2.038624	-1.001660	0.754917
4	6	0	3.400032	-1.249051	0.927941
5	6	0	4.508313	-0.560444	0.413707
6	6	0	4.508385	0.559727	-0.414955
7	6	0	1.387348	0.000526	0.000351
8	6	0	-0.095412	0.000336	0.000210
9	6	0	-0.836613	-1.183675	-0.177686
10	6	0	-0.837270	1.183945	0.177936
11	6	0	-2.226465	-1.195252	-0.189380

12	6	0	-2.227144	1.194822	0.189128
13	6	0	-2.925859	-0.000382	-0.000274
14	1	0	1.385234	-1.678743	1.296162
15	1	0	3.633392	-2.095738	1.569607
16	1	0	5.483063	-0.946987	0.701884
17	1	0	5.483196	0.945334	-0.704158
18	1	0	3.633615	2.096471	-1.568991
19	1	0	1.385445	1.680467	-1.294529
20	9	0	-0.196488	-2.345211	-0.391260
21	9	0	-2.888591	-2.331508	-0.387577
22	9	0	-4.249477	-0.000735	-0.000487
23	9	0	-2.889890	2.330742	0.387187
24	9	0	-0.197853	2.345792	0.391960

1e_carbene_s.log

SCF Done: E(RB3LYP) = -997.483291888 A.U. after 11 cycles

Zero-point correction= 0.143455
(Hartree/Particle)
Thermal correction to Energy= 0.158141
Thermal correction to Enthalpy= 0.159086
Thermal correction to Gibbs Free Energy= 0.100736
Sum of electronic and zero-point Energies= -997.339837
Sum of electronic and thermal Energies= -997.325151
Sum of electronic and thermal Enthalpies= -997.324206
Sum of electronic and thermal Free Energies= -997.382556

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	99.235	55.285	122.808

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.881144	1.347544	0.193683
2	6	0	0.578359	0.888523	0.349127
3	6	0	0.240494	-0.489892	0.307799
4	6	0	1.326234	-1.367937	0.045179
5	6	0	2.616522	-0.919392	-0.187506
6	6	0	2.902874	0.445497	-0.096761
7	6	0	-1.025513	-1.031765	0.716351
8	6	0	-2.251886	-0.486566	0.236600
9	6	0	-2.399815	0.220049	-0.993008
10	6	0	-3.426053	-0.754278	0.995907

11	6	0	-3.650740	0.631643	-1.430952
12	6	0	-4.667185	-0.281277	0.587256
13	6	0	-4.781468	0.399021	-0.632585
14	9	0	-0.363770	1.805476	0.641098
15	9	0	2.159084	2.657437	0.288972
16	9	0	4.151906	0.882791	-0.289929
17	9	0	3.602411	-1.783259	-0.472642
18	9	0	1.099412	-2.685941	-0.022430
19	1	0	-1.520771	0.411946	-1.601940
20	1	0	-3.755432	1.149090	-2.380881
21	1	0	-5.757155	0.738861	-0.971178
22	1	0	-5.550990	-0.466199	1.191515
23	1	0	-3.314839	-1.329256	1.910308

1e_carbene_t.log

SCF Done: E(UB3LYP) = -997.493466167 A.U. after 1 cycles

Zero-point correction= 0.142613
(Hartree/Particle)
Thermal correction to Energy= 0.157532
Thermal correction to Enthalpy= 0.158476
Thermal correction to Gibbs Free Energy= 0.098009
Sum of electronic and zero-point Energies= -997.350853
Sum of electronic and thermal Energies= -997.335935
Sum of electronic and thermal Enthalpies= -997.334990
Sum of electronic and thermal Free Energies= -997.395457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	98.853	55.797	127.262

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.076343	1.328464	-0.164995
2	6	0	0.740332	0.972622	-0.246123
3	6	0	0.297547	-0.378484	-0.130104
4	6	0	1.329780	-1.342409	0.062345
5	6	0	2.668288	-0.996845	0.138864
6	6	0	3.050344	0.343677	0.025293
7	6	0	-1.035361	-0.765754	-0.257667
8	6	0	-2.371640	-0.384154	-0.088672
9	6	0	-3.390480	-0.939700	-0.916927
10	6	0	-2.766224	0.521525	0.942672

11	6	0	-4.722119	-0.592172	-0.731719
12	6	0	-4.102578	0.858966	1.111322
13	6	0	-5.088230	0.308099	0.279353
14	9	0	-0.169330	1.942505	-0.440281
15	9	0	2.447977	2.613077	-0.274957
16	9	0	4.342632	0.682744	0.100238
17	9	0	3.606210	-1.937157	0.326865
18	9	0	0.994373	-2.636708	0.179551
19	1	0	-3.106164	-1.638930	-1.697816
20	1	0	-5.483576	-1.022587	-1.376898
21	1	0	-6.131773	0.575922	0.419825
22	1	0	-4.383320	1.555185	1.897516
23	1	0	-2.007949	0.947258	1.592769

1f+.log

SCF Done: E(RB3LYP) = -838.811631723 A.U. after 1 cycles

Zero-point correction= 0.203880
(Hartree/Particle)
Thermal correction to Energy= 0.217608
Thermal correction to Enthalpy= 0.218552
Thermal correction to Gibbs Free Energy= 0.160056
Sum of electronic and zero-point Energies= -838.607751
Sum of electronic and thermal Energies= -838.594024
Sum of electronic and thermal Enthalpies= -838.593080
Sum of electronic and thermal Free Energies= -838.651576

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.551	53.035	123.116

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.301281	0.440086	-0.298042
2	6	0	-4.084896	1.101101	-0.281041
3	6	0	-2.877177	0.400274	0.028450
4	6	0	-2.962291	-0.977326	0.398805
5	6	0	-4.186697	-1.620552	0.403721
6	6	0	-5.352285	-0.920759	0.040763
7	1	0	-6.210690	0.972576	-0.557663
8	1	0	-4.034513	2.156922	-0.533630
9	1	0	-2.079343	-1.504404	0.740710
10	1	0	-4.253462	-2.660801	0.706702

11	6	0	-1.675410	1.143049	-0.020517
12	1	0	-1.814320	2.224486	-0.042167
13	6	0	-0.313124	0.729534	-0.044905
14	6	0	0.127555	-0.574854	-0.411734
15	6	0	0.665294	1.709784	0.284006
16	6	0	1.475126	-0.885311	-0.395429
17	1	0	-0.581508	-1.311866	-0.769556
18	6	0	2.013832	1.385278	0.325621
19	1	0	0.347790	2.718260	0.534525
20	6	0	2.415743	0.087379	-0.010276
21	1	0	1.811196	-1.872970	-0.695287
22	1	0	2.750458	2.131150	0.602542
23	6	0	3.885800	-0.298782	-0.002709
24	9	0	4.087535	-1.358089	0.810193
25	9	0	4.671646	0.707229	0.418408
26	9	0	4.284376	-0.652519	-1.243459
27	1	0	-6.308749	-1.436346	0.047262

1fH.log

SCF Done: E(RB3LYP) = -839.695029863 A.U. after 1 cycles

Zero-point correction= 0.214270
(Hartree/Particle)
Thermal correction to Energy= 0.228333
Thermal correction to Enthalpy= 0.229277
Thermal correction to Gibbs Free Energy= 0.168044
Sum of electronic and zero-point Energies= -839.480760
Sum of electronic and thermal Energies= -839.466697
Sum of electronic and thermal Enthalpies= -839.465753
Sum of electronic and thermal Free Energies= -839.526986

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	143.281	53.969	128.876

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.985825	0.893960	1.447575
2	6	0	-2.968361	-0.017652	1.162356
3	6	0	-2.845243	-0.581190	-0.117554
4	6	0	-3.766805	-0.205887	-1.103409
5	6	0	-4.788002	0.708718	-0.822711
6	6	0	-4.900278	1.261663	0.454199

7	1	0	-4.065765	1.318414	2.445336
8	1	0	-2.258650	-0.292663	1.939951
9	1	0	-3.689585	-0.635400	-2.100468
10	1	0	-5.493090	0.986050	-1.602459
11	6	0	-1.742644	-1.583936	-0.419712
12	1	0	-1.851824	-2.457971	0.235296
13	1	0	-1.874117	-1.954867	-1.445079
14	6	0	-0.330381	-1.038864	-0.270228
15	6	0	0.613675	-1.698998	0.525244
16	6	0	0.066098	0.128563	-0.943381
17	6	0	1.920313	-1.218778	0.648057
18	1	0	0.328551	-2.602846	1.058821
19	6	0	1.365019	0.615696	-0.829860
20	1	0	-0.653994	0.666146	-1.555072
21	6	0	2.297399	-0.058209	-0.029587
22	1	0	2.635957	-1.743228	1.272826
23	1	0	1.654125	1.520960	-1.355685
24	6	0	3.706892	0.459293	0.052638
25	9	0	4.397438	-0.067625	1.093306
26	9	0	3.748942	1.810617	0.191075
27	9	0	4.421362	0.172232	-1.072296
28	1	0	-5.692440	1.972131	0.676002

1f+_troplium_1.log

SCF Done: E(RB3LYP) = -838.800542647 A.U. after 1 cycles

Zero-point correction= 0.204529
(Hartree/Particle)
Thermal correction to Energy= 0.218140
Thermal correction to Enthalpy= 0.219084
Thermal correction to Gibbs Free Energy= 0.162367
Sum of electronic and zero-point Energies= -838.596013
Sum of electronic and thermal Energies= -838.582403
Sum of electronic and thermal Enthalpies= -838.581459
Sum of electronic and thermal Free Energies= -838.638176

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.885	52.959	119.372

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.696611	2.092633	0.405313

2	6	0	1.946619	1.452728	0.279183
3	6	0	2.188683	0.114489	0.018042
4	6	0	-0.588274	1.579317	0.313138
5	6	0	1.230346	-0.903074	-0.180602
6	6	0	-1.032250	0.254887	0.050843
7	6	0	-0.154731	-0.839222	-0.172519
8	1	0	0.752026	3.156203	0.626410
9	1	0	-1.377111	2.302421	0.498401
10	1	0	1.638450	-1.889740	-0.387991
11	1	0	-0.643787	-1.781493	-0.400760
12	6	0	-2.479630	0.003334	0.008498
13	6	0	-3.012861	-1.224026	0.466909
14	6	0	-3.368891	0.983271	-0.491393
15	6	0	-4.384315	-1.453535	0.438495
16	1	0	-2.362360	-1.978834	0.899140
17	6	0	-4.736543	0.735894	-0.543773
18	1	0	-2.988135	1.917845	-0.893022
19	6	0	-5.248925	-0.478703	-0.072971
20	1	0	-4.781410	-2.389142	0.820348
21	1	0	-5.403796	1.486256	-0.956794
22	1	0	2.816730	2.089896	0.406793
23	6	0	3.644201	-0.355783	-0.081550
24	9	0	4.519615	0.639388	0.125241
25	9	0	3.878578	-1.321326	0.830622
26	9	0	3.875992	-0.876047	-1.304075
27	1	0	-6.318511	-0.664818	-0.104297

1f+_troplium_2.log

SCF Done: E(RB3LYP) = -838.807685407 A.U. after 11 cycles

Zero-point correction= 0.204575
(Hartree/Particle)
Thermal correction to Energy= 0.218262
Thermal correction to Enthalpy= 0.219207
Thermal correction to Gibbs Free Energy= 0.160992
Sum of electronic and zero-point Energies= -838.603110
Sum of electronic and thermal Energies= -838.589423
Sum of electronic and thermal Enthalpies= -838.588479
Sum of electronic and thermal Free Energies= -838.646693

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.962	52.936	122.523

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.978631	1.505847	0.406619
2	6	0	5.093525	0.677273	0.191862
3	6	0	5.098739	-0.666160	-0.165548
4	6	0	2.621357	1.209401	0.326216
5	6	0	3.990303	-1.499834	-0.393563
6	6	0	1.965540	-0.001647	-0.005539
7	6	0	2.630808	-1.209665	-0.329336
8	1	0	4.209479	2.529770	0.692687
9	1	0	1.962282	2.034618	0.581793
10	1	0	4.229259	-2.522692	-0.676776
11	1	0	1.978706	-2.037973	-0.592632
12	6	0	0.486452	-0.004763	-0.013904
13	6	0	-0.232682	-1.121060	0.460864
14	6	0	-0.231480	1.107665	-0.498551
15	6	0	-1.623775	-1.118937	0.463266
16	1	0	0.290061	-1.978282	0.875187
17	6	0	-1.622851	1.099705	-0.518496
18	1	0	0.292655	1.965234	-0.910442
19	6	0	-2.319895	-0.011213	-0.032557
20	1	0	-2.166008	-1.975816	0.849375
21	1	0	-2.163712	1.949811	-0.920671
22	1	0	6.074642	-1.130244	-0.287649
23	6	0	-3.834798	0.001331	0.004208
24	9	0	-4.344998	-1.237856	-0.157768
25	9	0	-4.350710	0.791393	-0.960239
26	9	0	-4.279001	0.470032	1.194702
27	1	0	6.065769	1.145806	0.325626

1f_carbene_s.log

SCF Done: E(RB3LYP) = -838.375484803 A.U. after 11 cycles

Zero-point correction= 0.189148
(Hartree/Particle)
Thermal correction to Energy= 0.202902
Thermal correction to Enthalpy= 0.203846
Thermal correction to Gibbs Free Energy= 0.145241
Sum of electronic and zero-point Energies= -838.186337
Sum of electronic and thermal Energies= -838.172583
Sum of electronic and thermal Enthalpies= -838.171639
Sum of electronic and thermal Free Energies= -838.230244

E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin

Total 127.323 53.005 123.345

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.194212	0.124679	0.534311
2	6	0	4.069858	0.939121	0.597416
3	6	0	2.835042	0.532641	0.019207
4	6	0	2.807252	-0.704347	-0.688874
5	6	0	3.954168	-1.482089	-0.809369
6	6	0	5.141122	-1.079727	-0.181989
7	1	0	6.122170	0.434706	1.007318
8	1	0	4.099376	1.900768	1.101348
9	1	0	1.885170	-1.018337	-1.169115
10	1	0	3.928403	-2.408625	-1.377364
11	6	0	1.720577	1.424331	0.127889
12	6	0	0.385001	0.907255	0.067530
13	6	0	-0.028736	-0.264467	0.759407
14	6	0	-0.611075	1.651726	-0.622237
15	6	0	-1.363574	-0.659730	0.767549
16	1	0	0.702396	-0.835110	1.324122
17	6	0	-1.923898	1.209579	-0.681595
18	1	0	-0.316712	2.572984	-1.115919
19	6	0	-2.308806	0.058845	0.027331
20	1	0	-1.665754	-1.542416	1.322192
21	1	0	-2.663454	1.771360	-1.244467
22	6	0	-3.756041	-0.351359	0.027747
23	9	0	-3.936235	-1.628166	0.445011
24	9	0	-4.312544	-0.253972	-1.207971
25	9	0	-4.508284	0.435951	0.846408
26	1	0	6.031361	-1.698393	-0.265084

1f_carbene_t.log

SCF Done: E(UB3LYP) = -838.384444837 A.U. after 11 cycles

Zero-point correction= 0.188265
(Hartree/Particle)
Thermal correction to Energy= 0.202223
Thermal correction to Enthalpy= 0.203167
Thermal correction to Gibbs Free Energy= 0.142491
Sum of electronic and zero-point Energies= -838.196179
Sum of electronic and thermal Energies= -838.182222
Sum of electronic and thermal Enthalpies= -838.181278
Sum of electronic and thermal Free Energies= -838.241954

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.897	53.448	127.704

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.310612	-0.502483	-0.608358
2	6	0	4.036817	-1.057142	-0.603702
3	6	0	2.950673	-0.383892	0.026479
4	6	0	3.221138	0.863817	0.666444
5	6	0	4.500626	1.405802	0.649570
6	6	0	5.552523	0.730869	0.013759
7	1	0	6.123850	-1.030561	-1.099737
8	1	0	3.850436	-2.012761	-1.085466
9	1	0	2.413663	1.382408	1.175573
10	1	0	4.685063	2.358683	1.139593
11	6	0	1.668139	-0.956215	0.057981
12	6	0	0.304223	-0.642984	0.054875
13	6	0	-0.179035	0.587584	-0.490984
14	6	0	-0.661276	-1.561813	0.564400
15	6	0	-1.534364	0.878139	-0.503166
16	1	0	0.530958	1.297365	-0.904631
17	6	0	-2.014383	-1.262934	0.543224
18	1	0	-0.317893	-2.505069	0.978390
19	6	0	-2.461693	-0.040145	0.015976
20	1	0	-1.879929	1.820808	-0.916573
21	1	0	-2.730725	-1.973410	0.943863
22	6	0	-3.932061	0.257257	-0.052001
23	9	0	-4.193612	1.587566	0.016051
24	9	0	-4.626502	-0.337645	0.950922
25	9	0	-4.490787	-0.182349	-1.216483
26	1	0	6.551036	1.159224	0.007602

1g+.log

SCF Done: E(RB3LYP) = -799.472366278 A.U. after 1 cycles

Zero-point correction= 0.174635
(Hartree/Particle)
Thermal correction to Energy= 0.187148
Thermal correction to Enthalpy= 0.188093
Thermal correction to Gibbs Free Energy= 0.134455
Sum of electronic and zero-point Energies= -799.297731

Sum of electronic and thermal Energies= -799.285218
Sum of electronic and thermal Enthalpies= -799.284274
Sum of electronic and thermal Free Energies= -799.337911

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.437	49.081	112.889

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.505971	0.801416	0.203538
2	6	0	-2.243707	1.361704	0.097307
3	6	0	-1.126214	0.510907	-0.126125
4	6	0	-1.332851	-0.883499	-0.305423
5	6	0	-2.621274	-1.378610	-0.217310
6	6	0	-3.727716	-0.566629	0.048309
7	6	0	0.153115	1.143218	-0.190584
8	1	0	0.108661	2.217131	-0.371701
9	6	0	1.456319	0.625949	-0.058150
10	6	0	2.538521	1.476893	-0.458729
11	6	0	1.769847	-0.663526	0.481606
12	6	0	3.847466	1.045378	-0.403175
13	6	0	3.076899	-1.092949	0.562377
14	6	0	4.092998	-0.238463	0.101927
15	1	0	-0.531793	-1.556520	-0.582580
16	1	0	-4.727827	-0.984175	0.106843
17	1	0	-2.122682	2.433897	0.213061
18	1	0	0.984811	-1.288691	0.889696
19	1	0	4.677338	1.666505	-0.723352
20	1	0	2.317619	2.469963	-0.840183
21	1	0	3.342296	-2.054817	0.988646
22	9	0	-4.554962	1.597007	0.442840
23	9	0	-2.827614	-2.688260	-0.408400
24	9	0	5.347796	-0.659193	0.177357

1gH.log

SCF Done: E(RB3LYP) = -799.472366278 A.U. after 1 cycles

Zero-point correction= 0.174635
(Hartree/Particle)
Thermal correction to Energy= 0.187148
Thermal correction to Enthalpy= 0.188093
Thermal correction to Gibbs Free Energy= 0.134455

Sum of electronic and zero-point Energies= -799.297731
Sum of electronic and thermal Energies= -799.285218
Sum of electronic and thermal Enthalpies= -799.284274
Sum of electronic and thermal Free Energies= -799.337911

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.437	49.081	112.889

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.505971	0.801416	0.203538
2	6	0	-2.243707	1.361704	0.097307
3	6	0	-1.126214	0.510907	-0.126125
4	6	0	-1.332851	-0.883499	-0.305423
5	6	0	-2.621274	-1.378610	-0.217310
6	6	0	-3.727716	-0.566629	0.048309
7	6	0	0.153115	1.143218	-0.190584
8	1	0	0.108661	2.217131	-0.371701
9	6	0	1.456319	0.625949	-0.058150
10	6	0	2.538521	1.476893	-0.458729
11	6	0	1.769847	-0.663526	0.481606
12	6	0	3.847466	1.045378	-0.403175
13	6	0	3.076899	-1.092949	0.562377
14	6	0	4.092998	-0.238463	0.101927
15	1	0	-0.531793	-1.556520	-0.582580
16	1	0	-4.727827	-0.984175	0.106843
17	1	0	-2.122682	2.433897	0.213061
18	1	0	0.984811	-1.288691	0.889696
19	1	0	4.677338	1.666505	-0.723352
20	1	0	2.317619	2.469963	-0.840183
21	1	0	3.342296	-2.054817	0.988646
22	9	0	-4.554962	1.597007	0.442840
23	9	0	-2.827614	-2.688260	-0.408400
24	9	0	5.347796	-0.659193	0.177357

1g_tropylium_1.log

SCF Done: E(RB3LYP) = -799.466680294 A.U. after 1 cycles

Zero-point correction= 0.175195
(Hartree/Particle)
Thermal correction to Energy= 0.187647
Thermal correction to Enthalpy= 0.188591

Thermal correction to Gibbs Free Energy= 0.135484
Sum of electronic and zero-point Energies= -799.291486
Sum of electronic and thermal Energies= -799.279033
Sum of electronic and thermal Enthalpies= -799.278089
Sum of electronic and thermal Free Energies= -799.331196

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.750	48.949	111.773

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.733378	1.186549	-0.545777
2	6	0	1.368282	0.981200	-0.450170
3	6	0	1.212739	-1.293543	0.589850
4	6	0	2.556553	-1.648208	0.733779
5	6	0	3.716624	-0.942124	0.404969
6	6	0	3.775004	0.323680	-0.165040
7	1	0	0.766232	1.791648	-0.850957
8	1	0	2.728028	-2.622581	1.185527
9	6	0	0.631016	-0.124388	0.057169
10	6	0	-0.845778	-0.035832	0.020475
11	6	0	-1.615379	-1.179167	-0.272138
12	6	0	-1.489259	1.190450	0.280632
13	6	0	-2.999589	-1.064207	-0.306485
14	1	0	-1.166351	-2.133225	-0.525838
15	6	0	-2.877737	1.237010	0.255259
16	1	0	-0.945240	2.087643	0.555417
17	6	0	-3.665526	0.128806	-0.041417
18	1	0	-4.747925	0.192168	-0.066054
19	1	0	0.510466	-2.029720	0.970343
20	9	0	-3.725132	-2.151090	-0.613539
21	9	0	-3.484535	2.401947	0.532268
22	9	0	4.999989	0.797782	-0.392420
23	1	0	4.675621	-1.410547	0.611957
24	1	0	3.064305	2.125511	-0.983814

1g_tropylium_2.log

SCF Done: E(RB3LYP) = -799.469612397 A.U. after 1 cycles

Zero-point correction= 0.175215
(Hartree/Particle)
Thermal correction to Energy= 0.187615

```
 Thermal correction to Enthalpy=                  0.188559
 Thermal correction to Gibbs Free Energy=         0.135588
 Sum of electronic and zero-point Energies=           -799.294397
 Sum of electronic and thermal Energies=              -799.281998
 Sum of electronic and thermal Enthalpies=            -799.281053
 Sum of electronic and thermal Free Energies=         -799.334024

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 117.730             48.800            111.486


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.303963    1.375325   -0.188176
      2          6           0        0.936447    1.114606   -0.168556
      3          6           0        0.917430   -1.368094    0.184715
      4          6           0        2.255905   -1.687331    0.228003
      5          6           0        3.370882   -0.825978    0.115322
      6          6           0        3.421366    0.539736   -0.068191
      7          1           0        0.329865    1.998174   -0.343216
      8          1           0        2.515078   -2.731410    0.387063
      9          6           0        0.261705   -0.107273    0.006664
     10          6           0       -1.208036   -0.093305    0.013349
     11          6           0       -1.946849   -1.177027   -0.518455
     12          6           0       -1.917754    1.009063    0.546219
     13          6           0       -3.334969   -1.157748   -0.534943
     14          1           0       -1.438742   -2.020828   -0.975478
     15          6           0       -3.305595    1.029007    0.559203
     16          1           0       -1.384778    1.836680    1.004638
     17          6           0       -3.991968   -0.054935    0.010948
     18          1           0        0.252716   -2.211904    0.340963
     19          9           0        4.550166   -1.439849    0.208668
     20          9           0        2.614666    2.661159   -0.377751
     21          9           0       -5.329207   -0.036962    0.010756
     22          1           0        4.400203    1.007839   -0.130626
     23          1           0       -3.910728   -1.969870   -0.966163
     24          1           0       -3.859399    1.855904    0.991151
 ---------------------------------------------------------------------
```

1g_carbene_s.log

```
 SCF Done:  E(RB3LYP) =  -799.040798958     A.U. after   11 cycles

 Zero-point correction=                           0.159958
(Hartree/Particle)
```

```
 Thermal correction to Energy=                    0.172532
 Thermal correction to Enthalpy=                  0.173476
 Thermal correction to Gibbs Free Energy=         0.119643
 Sum of electronic and zero-point Energies=           -798.880841
 Sum of electronic and thermal Energies=              -798.868267
 Sum of electronic and thermal Enthalpies=            -798.867323
 Sum of electronic and thermal Free Energies=         -798.921156

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 108.265             49.143           113.302
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.503338	1.335673	0.363294
2	6	0	-1.255151	0.770460	0.571781
3	6	0	-1.079699	-0.622145	0.339576
4	6	0	-2.190438	-1.380621	-0.116924
5	6	0	-3.382628	-0.734804	-0.386312
6	6	0	-3.588156	0.622677	-0.137085
7	6	0	0.139718	-1.315863	0.650084
8	6	0	1.396409	-0.728818	0.302686
9	6	0	2.548439	-1.171290	1.013718
10	6	0	1.590649	0.213737	-0.751097
11	6	0	3.809917	-0.658623	0.746284
12	6	0	2.856605	0.684868	-1.073355
13	6	0	3.936218	0.252561	-0.302803
14	1	0	2.406447	-1.918665	1.788292
15	1	0	0.735596	0.539993	-1.334841
16	1	0	-0.444455	1.383564	0.949479
17	1	0	-2.098772	-2.452510	-0.252015
18	9	0	-2.675092	2.657519	0.623992
19	9	0	-4.428532	-1.454722	-0.864796
20	9	0	5.166374	0.723582	-0.600642
21	1	0	4.690911	-0.968455	1.299136
22	1	0	3.024561	1.379236	-1.890791
23	1	0	-4.550305	1.092546	-0.305324

1g_carbene_t.log

```
 SCF Done:  E(UB3LYP) =  -799.047639336     A.U. after    1 cycles

 Zero-point correction=                           0.159017
(Hartree/Particle)
```

Thermal correction to Energy= 0.171810
Thermal correction to Enthalpy= 0.172754
Thermal correction to Gibbs Free Energy= 0.116842
Sum of electronic and zero-point Energies= -798.888622
Sum of electronic and thermal Energies= -798.875829
Sum of electronic and thermal Enthalpies= -798.874885
Sum of electronic and thermal Free Energies= -798.930797

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	107.812	49.666	117.677

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.755650	1.331829	0.277756
2	6	0	-1.444730	0.901018	0.350534
3	6	0	-1.153347	-0.476640	0.105169
4	6	0	-2.234873	-1.357732	-0.189165
5	6	0	-3.519863	-0.852438	-0.237504
6	6	0	-3.828707	0.489471	-0.013364
7	6	0	0.158429	-0.964562	0.187200
8	6	0	1.502419	-0.565771	0.095820
9	6	0	2.511718	-1.220914	0.859865
10	6	0	1.912980	0.468882	-0.799308
11	6	0	3.847035	-0.855138	0.752144
12	6	0	3.248021	0.838595	-0.903825
13	6	0	4.192217	0.171094	-0.125767
14	1	0	2.221507	-2.017530	1.538238
15	1	0	1.167541	0.967147	-1.411791
16	1	0	-0.657258	1.602168	0.602976
17	1	0	-2.054624	-2.410202	-0.376740
18	9	0	-3.024200	2.642617	0.508272
19	9	0	-4.542515	-1.697844	-0.522723
20	9	0	5.496708	0.530384	-0.230703
21	1	0	4.619233	-1.347384	1.334963
22	1	0	3.566786	1.626388	-1.579424
23	1	0	-4.847015	0.856834	-0.059153

2.log

SCF Done: E(RB3LYP) = -601.611218284 A.U. after 1 cycles

Zero-point correction= 0.173577
(Hartree/Particle)

Thermal correction to Energy= 0.184011
Thermal correction to Enthalpy= 0.184956
Thermal correction to Gibbs Free Energy= 0.136678
Sum of electronic and zero-point Energies= -601.437641
Sum of electronic and thermal Energies= -601.427207
Sum of electronic and thermal Enthalpies= -601.426263
Sum of electronic and thermal Free Energies= -601.474541

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	115.469	38.699	101.610

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.644193	-0.437706	-0.000072
2	1	0	1.861985	-1.914371	-0.000306
3	6	0	2.433536	0.305546	1.551764
4	1	0	2.007995	-0.134375	2.461581
5	1	0	3.516309	0.127396	1.566046
6	1	0	2.274481	1.390274	1.602014
7	6	0	2.433758	0.306072	-1.551536
8	1	0	3.516508	0.127791	-1.565794
9	1	0	2.008245	-0.133435	-2.461568
10	1	0	2.274855	1.390842	-1.601378
11	6	0	-0.226990	-0.168630	-0.000091
12	6	0	-1.117884	-1.258269	-0.000197
13	6	0	-0.783665	1.125752	0.000079
14	6	0	-2.503639	-1.067674	-0.000134
15	1	0	-0.726152	-2.273668	-0.000347
16	6	0	-2.166479	1.325157	0.000145
17	1	0	-0.132273	1.998776	0.000147
18	6	0	-3.031008	0.225921	0.000046
19	1	0	-3.169201	-1.927823	-0.000224
20	1	0	-2.569535	2.335302	0.000273
21	1	0	-4.107691	0.377924	0.000114

2+.log

SCF Done: E(RB3LYP) = -600.742980759 A.U. after 1 cycles

Zero-point correction= 0.165212
(Hartree/Particle)
Thermal correction to Energy= 0.175724
Thermal correction to Enthalpy= 0.176668

```
 Thermal correction to Gibbs Free Energy=         0.127834
 Sum of electronic and zero-point Energies=           -600.577768
 Sum of electronic and thermal Energies=              -600.567257
 Sum of electronic and thermal Enthalpies=            -600.566312
 Sum of electronic and thermal Free Energies=         -600.615147

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 110.269             37.398            102.780


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.548857    1.583051   -0.001013
      2          1           0        3.408471    1.503894   -0.678251
      3          1           0        1.952121    2.453281   -0.287777
      4          1           0        2.956259    1.767279    1.004157
      5          6           0        2.548812   -1.583070    0.000999
      6          1           0        3.408582   -1.503874    0.678032
      7          1           0        1.952095   -2.453236    0.288001
      8          1           0        2.955971   -1.767451   -1.004242
      9         14           0        1.587431    0.000005    0.000005
     10          6           0       -0.218019    0.000003    0.000015
     11          6           0       -0.942053   -1.223217    0.002492
     12          6           0       -0.942054    1.223223   -0.002471
     13          6           0       -2.331703   -1.218359    0.001006
     14          1           0       -0.418132   -2.174880    0.004582
     15          6           0       -2.331704    1.218368   -0.001013
     16          1           0       -0.418129    2.174885   -0.004549
     17          6           0       -3.024353    0.000004   -0.000011
     18          1           0       -2.878567   -2.156271    0.001660
     19          1           0       -2.878568    2.156279   -0.001680
     20          1           0       -4.110829    0.000004   -0.000023
 ---------------------------------------------------------------------
```

3.log

```
 SCF Done:  E(RB3LYP) =  -645.735360586     A.U. after    1 cycles


 Zero-point correction=                           0.291469
(Hartree/Particle)
 Thermal correction to Energy=                    0.306832
 Thermal correction to Enthalpy=                  0.307776
 Thermal correction to Gibbs Free Energy=         0.249795
 Sum of electronic and zero-point Energies=           -645.443891
 Sum of electronic and thermal Energies=              -645.428529
```

Sum of electronic and thermal Enthalpies= -645.427584
Sum of electronic and thermal Free Energies= -645.485566

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.540	55.877	122.032

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.037414	-0.056934	-0.509909
2	1	0	0.155178	-0.110606	-1.994604
3	6	0	-1.876135	-0.498145	-0.190158
4	1	0	-1.995551	-1.517020	-0.591349
5	6	0	-2.835924	0.414396	-0.979883
6	1	0	-2.610683	0.415972	-2.053444
7	1	0	-3.877739	0.084040	-0.860664
8	1	0	-2.787263	1.453793	-0.629118
9	6	0	0.360812	1.734272	0.065715
10	1	0	-0.589286	2.281823	-0.041944
11	6	0	0.778238	1.832809	1.547964
12	1	0	0.907491	2.882910	1.846514
13	1	0	0.036010	1.390148	2.222868
14	1	0	1.733784	1.325722	1.732376
15	6	0	1.128718	-1.369291	0.260258
16	1	0	1.056799	-1.263810	1.354435
17	6	0	0.696362	-2.805496	-0.099906
18	1	0	1.382723	-3.541386	0.343019
19	1	0	-0.311741	-3.041161	0.260601
20	1	0	0.706620	-2.966520	-1.186426
21	6	0	1.390347	2.443112	-0.838760
22	1	0	1.075776	2.449820	-1.888880
23	1	0	1.530138	3.487875	-0.525590
24	1	0	2.373795	1.958310	-0.794166
25	6	0	2.602726	-1.143627	-0.135059
26	1	0	2.738936	-1.213143	-1.222357
27	1	0	2.975608	-0.163129	0.182364
28	1	0	3.250753	-1.904152	0.323886
29	6	0	-2.263238	-0.537492	1.301598
30	1	0	-2.193530	0.457130	1.761069
31	1	0	-3.301135	-0.877106	1.428446
32	1	0	-1.624327	-1.215656	1.881077

3+.log

SCF Done: E(RB3LYP) = -644.864248664 A.U. after 7 cycles

Zero-point correction=	0.282892
(Hartree/Particle)	
Thermal correction to Energy=	0.298783
Thermal correction to Enthalpy=	0.299727
Thermal correction to Gibbs Free Energy=	0.238646
Sum of electronic and zero-point Energies=	-644.581357
Sum of electronic and thermal Energies=	-644.565466
Sum of electronic and thermal Enthalpies=	-644.564522
Sum of electronic and thermal Free Energies=	-644.625603

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.489	55.195	128.556

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.142729	-0.140448	0.027332
2	6	0	-0.264417	1.672700	-0.224984
3	1	0	0.686687	2.155260	-0.488400
4	6	0	-1.257372	1.884335	-1.397698
5	1	0	-2.233354	1.429831	-1.197480
6	1	0	-1.420144	2.960274	-1.531301
7	1	0	-0.881627	1.493907	-2.350354
8	6	0	-1.154007	-1.457294	0.320901
9	1	0	-0.651128	-2.228657	0.923763
10	6	0	-1.432180	-2.084022	-1.084187
11	1	0	-2.088753	-2.951881	-0.950652
12	1	0	-1.949623	-1.385365	-1.751079
13	1	0	-0.527377	-2.445440	-1.588566
14	6	0	1.925916	-0.704280	-0.014082
15	1	0	1.911292	-1.796987	-0.129461
16	6	0	2.783077	-0.083541	-1.137310
17	1	0	3.807456	-0.466903	-1.063970
18	1	0	2.411096	-0.335409	-2.136435
19	1	0	2.838771	1.007739	-1.056224
20	6	0	-2.456190	-1.033613	1.025919
21	1	0	-3.004117	-0.275450	0.456675
22	1	0	-3.114239	-1.904842	1.123352
23	1	0	-2.276989	-0.645019	2.033607
24	6	0	-0.786955	2.317428	1.088084
25	1	0	-0.080567	2.225015	1.921226
26	1	0	-0.940831	3.388964	0.913909
27	1	0	-1.747233	1.894536	1.399492
28	6	0	2.510312	-0.382693	1.397103
29	1	0	1.955406	-0.856150	2.216704
30	1	0	3.536206	-0.767298	1.444063
31	1	0	2.561749	0.696021	1.586014

4.log

SCF Done: E(RB3LYP) = -527.802081838 A.U. after 1 cycles

Zero-point correction= 0.205945
(Hartree/Particle)
Thermal correction to Energy= 0.217545
Thermal correction to Enthalpy= 0.218489
Thermal correction to Gibbs Free Energy= 0.167796
Sum of electronic and zero-point Energies= -527.596136
Sum of electronic and thermal Energies= -527.584537
Sum of electronic and thermal Enthalpies= -527.583593
Sum of electronic and thermal Free Energies= -527.634286

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	136.511	40.012	106.693

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.193489	2.904878	0.163630
2	1	0	0.845411	3.005766	-0.173492
3	1	0	-0.187148	2.941786	1.260175
4	1	0	-0.737420	3.789867	-0.191222
5	6	0	-0.835779	1.602456	-0.350751
6	14	0	-0.000140	0.000060	0.244669
7	1	0	0.000145	0.001454	1.742938
8	6	0	-0.969422	-1.526432	-0.348127
9	6	0	-2.420151	-1.619203	0.162201
10	1	0	-2.458622	-1.629127	1.258627
11	1	0	-3.025520	-0.770690	-0.179463
12	1	0	-2.913859	-2.533529	-0.191507
13	6	0	1.805499	-0.077466	-0.350740
14	6	0	2.613387	-1.284550	0.163270
15	1	0	2.645617	-1.307099	1.259770
16	1	0	2.179951	-2.234977	-0.171449
17	1	0	3.650617	-1.256695	-0.194855
18	1	0	-0.961863	-1.539248	-1.448681
19	1	0	-0.845262	1.603159	-1.451422
20	1	0	1.810471	-0.069484	-1.451524
21	1	0	-0.415783	-2.424425	-0.038180
22	1	0	2.306723	0.852647	-0.046170
23	1	0	-1.891770	1.571654	-0.045815

4+.log

SCF Done: E(RB3LYP) = -526.924621413 A.U. after 7 cycles

Zero-point correction= 0.197197
(Hartree/Particle)
Thermal correction to Energy= 0.208891
Thermal correction to Enthalpy= 0.209835
Thermal correction to Gibbs Free Energy= 0.158121
Sum of electronic and zero-point Energies= -526.727424
Sum of electronic and thermal Energies= -526.715731
Sum of electronic and thermal Enthalpies= -526.714786
Sum of electronic and thermal Free Energies= -526.766500

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	131.081	39.043	108.841

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.117551	-0.105899	0.264115
2	6	0	-0.168877	1.679304	-0.160959
3	1	0	0.561108	2.261774	0.425072
4	1	0	0.180620	1.801126	-1.201586
5	6	0	-1.595732	2.236960	0.011486
6	1	0	-1.928696	2.190169	1.053112
7	1	0	-1.619154	3.287579	-0.292974
8	1	0	-2.323407	1.700489	-0.605394
9	6	0	-1.301665	-1.246128	0.626149
10	1	0	-0.960525	-2.073136	1.260538
11	1	0	-2.081281	-0.704188	1.175469
12	6	0	-1.895611	-1.810627	-0.704372
13	1	0	-2.732190	-2.472182	-0.459345
14	1	0	-2.283652	-1.020960	-1.356081
15	1	0	-1.166124	-2.401863	-1.267689
16	6	0	1.842055	-0.796656	0.243712
17	1	0	2.063091	-1.057599	1.294847
18	1	0	1.788699	-1.774675	-0.261197
19	6	0	2.964774	0.080577	-0.345895
20	1	0	3.921645	-0.443647	-0.264831
21	1	0	2.798498	0.298058	-1.405676
22	1	0	3.065990	1.031063	0.187399

5.log

SCF Done: E(RB3LYP) = -854.545562310 A.U. after 1 cycles

Zero-point correction= 0.198879
(Hartree/Particle)
Thermal correction to Energy= 0.213717
Thermal correction to Enthalpy= 0.214662
Thermal correction to Gibbs Free Energy= 0.154358
Sum of electronic and zero-point Energies= -854.346683
Sum of electronic and thermal Energies= -854.331845
Sum of electronic and thermal Enthalpies= -854.330901
Sum of electronic and thermal Free Energies= -854.391204

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.110	50.882	126.919

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.356711	-1.410016	0.000000
2	8	0	-0.141401	0.171511	0.000000
3	14	0	-0.826441	1.672399	-0.000000
4	6	0	2.243514	-1.431651	-0.000000
5	1	0	2.645890	-0.924217	0.885865
6	1	0	2.631399	-2.458927	-0.000000
7	1	0	2.645890	-0.924217	-0.885865
8	6	0	-0.310048	-2.258147	1.548871
9	1	0	0.056173	-1.767199	2.459426
10	1	0	-1.406844	-2.232238	1.574634
11	1	0	-0.001443	-3.311098	1.592025
12	6	0	-0.310048	-2.258147	-1.548871
13	1	0	0.056173	-1.767199	-2.459426
14	1	0	-0.001443	-3.311098	-1.592025
15	1	0	-1.406844	-2.232238	-1.574634
16	6	0	-0.310048	2.604196	-1.553685
17	1	0	0.777404	2.747437	-1.589412
18	1	0	-0.606899	2.059738	-2.458442
19	1	0	-0.780458	3.595674	-1.591782
20	6	0	-0.310048	2.604196	1.553685
21	1	0	-0.606899	2.059738	2.458442
22	1	0	0.777404	2.747437	1.589412
23	1	0	-0.780458	3.595674	1.591782
24	1	0	-2.311558	1.514608	0.000000

5+.log

SCF Done: E(RB3LYP) = -853.679387268 A.U. after 8 cycles

Zero-point correction= 0.190571
(Hartree/Particle)
Thermal correction to Energy= 0.205478
Thermal correction to Enthalpy= 0.206422
Thermal correction to Gibbs Free Energy= 0.146244
Sum of electronic and zero-point Energies= -853.488816
Sum of electronic and thermal Energies= -853.473909
Sum of electronic and thermal Enthalpies= -853.472965
Sum of electronic and thermal Free Energies= -853.533144

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	128.939	49.491	126.656

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.532606	-0.002314	-0.000116
2	8	0	-0.229322	-0.020648	0.002338
3	14	0	-1.799214	0.001076	0.000115
4	6	0	2.008933	-1.093532	-1.442881
5	1	0	1.629628	-0.703554	-2.394955
6	1	0	3.102060	-1.146537	-1.527682
7	1	0	1.642324	-2.119376	-1.319537
8	6	0	2.010502	1.791986	-0.226040
9	1	0	1.640632	2.199382	-1.174567
10	1	0	1.636724	2.422400	0.589583
11	1	0	3.103688	1.891267	-0.236544
12	6	0	2.002570	-0.700879	1.670546
13	1	0	1.636231	-1.725454	1.804762
14	1	0	3.095386	-0.730799	1.769449
15	1	0	1.620116	-0.086526	2.494331
16	6	0	-2.712600	-1.601849	0.004314
17	1	0	-2.126668	-2.392449	0.483751
18	1	0	-3.682577	-1.502946	0.504863
19	1	0	-2.908867	-1.913041	-1.032521
20	6	0	-2.678255	1.623206	-0.007314
21	1	0	-2.973308	1.884470	1.019835
22	1	0	-2.037526	2.423954	-0.388829
23	1	0	-3.597650	1.568128	-0.602379

TMS.log

SCF Done: E(RB3LYP) = -409.871433213 A.U. after 1 cycles

Zero-point correction= 0.119326
(Hartree/Particle)
Thermal correction to Energy= 0.126836
Thermal correction to Enthalpy= 0.127780
Thermal correction to Gibbs Free Energy= 0.089999
Sum of electronic and zero-point Energies= -409.752107
Sum of electronic and thermal Energies= -409.744598
Sum of electronic and thermal Enthalpies= -409.743653
Sum of electronic and thermal Free Energies= -409.781434

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.591	26.012	79.517

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.000000	-0.000000	0.377131
2	1	0	-0.000000	-0.000000	1.872092
3	6	0	-0.000000	1.796272	-0.222767
4	1	0	-0.885135	2.336381	0.135923
5	1	0	0.885135	2.336381	0.135923
6	1	0	-0.000000	1.850016	-1.319219
7	6	0	-1.555617	-0.898136	-0.222767
8	1	0	-2.465933	-0.401641	0.135923
9	1	0	-1.602161	-0.925008	-1.319219
10	1	0	-1.580797	-1.934740	0.135923
11	6	0	1.555617	-0.898136	-0.222767
12	1	0	2.465933	-0.401641	0.135923
13	1	0	1.580797	-1.934740	0.135923
14	1	0	1.602161	-0.925008	-1.319219

TMS+.log

SCF Done: E(RB3LYP) = -408.985707873 A.U. after 6 cycles

```
 Zero-point correction=                           0.109742
(Hartree/Particle)
 Thermal correction to Energy=                    0.117608
 Thermal correction to Enthalpy=                  0.118552
 Thermal correction to Gibbs Free Energy=         0.077038
 Sum of electronic and zero-point Energies=           -408.875966
 Sum of electronic and thermal Energies=              -408.868100
 Sum of electronic and thermal Enthalpies=            -408.867156
 Sum of electronic and thermal Free Energies=         -408.908670

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  73.800             24.847            87.373


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -0.000018    0.000001    0.000000
      2          6           0        0.881365    1.619608    0.000000
      3          1           0        1.969886    1.511843    0.000005
      4          1           0        0.581463    2.210864   -0.878113
      5          1           0        0.581454    2.210870    0.878106
      6          6           0       -1.843323   -0.046539    0.000000
      7          1           0       -2.294288    0.950016    0.000013
      8          1           0       -2.205393   -0.601902   -0.878113
      9          1           0       -2.205394   -0.601926    0.878098
     10          6           0        0.961973   -1.573071   -0.000000
     11          1           0        0.324479   -2.461942   -0.000012
     12          1           0        1.623988   -1.608905   -0.878100
     13          1           0        1.623968   -1.608916    0.878115
 ---------------------------------------------------------------------
```

H-.log

```
 SCF Done:  E(RB3LYP) = -0.461816668117     A.U. after    1 cycles


 Zero-point correction=                           0.000000
(Hartree/Particle)
 Thermal correction to Energy=                    0.001416
 Thermal correction to Enthalpy=                  0.002360
 Thermal correction to Gibbs Free Energy=        -0.010000
 Sum of electronic and zero-point Energies=             -0.461817
 Sum of electronic and thermal Energies=                -0.460400
 Sum of electronic and thermal Enthalpies=              -0.459456
 Sum of electronic and thermal Free Energies=           -0.471816
```

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	0.889	2.981	26.014

H2.log

SCF Done: E(RB3LYP) = -1.17548240892 A.U. after 1 cycles

Zero-point correction= 0.010145
(Hartree/Particle)
Thermal correction to Energy= 0.012505
Thermal correction to Enthalpy= 0.013450
Thermal correction to Gibbs Free Energy= -0.001342
Sum of electronic and zero-point Energies= -1.165337
Sum of electronic and thermal Energies= -1.162977
Sum of electronic and thermal Enthalpies= -1.162033
Sum of electronic and thermal Free Energies= -1.176825

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	7.847	4.968	31.132

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.371394
2	1	0	0.000000	0.000000	-0.371394

toluene.log

SCF Done: E(RB3LYP) = -271.577271836 A.U. after 1 cycles

Zero-point correction= 0.127991
(Hartree/Particle)
Thermal correction to Energy= 0.134225
Thermal correction to Enthalpy= 0.135169
Thermal correction to Gibbs Free Energy= 0.097145
Sum of electronic and zero-point Energies= -271.449281
Sum of electronic and thermal Energies= -271.443047
Sum of electronic and thermal Enthalpies= -271.442102
Sum of electronic and thermal Free Energies= -271.480127

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.228	23.222	80.029

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.202687	-1.206749	0.002100
2	6	0	-0.194899	-1.203491	-0.009423
3	6	0	-0.915815	0.000000	-0.011992
4	6	0	-0.194899	1.203491	-0.009423
5	6	0	1.202687	1.206749	0.002100
6	6	0	1.907831	0.000000	0.008939
7	1	0	1.740189	-2.152168	0.001925
8	1	0	-0.734196	-2.149012	-0.018569
9	1	0	-0.734196	2.149012	-0.018569
10	1	0	1.740189	2.152168	0.001925
11	1	0	2.994993	0.000000	0.015011
12	6	0	-2.428193	0.000000	0.009999
13	1	0	-2.809163	0.000000	1.040642
14	1	0	-2.837110	0.886387	-0.488087
15	1	0	-2.837110	-0.886387	-0.488087

benzyl-cation.log

SCF Done: E(RB3LYP) = -270.666649192 A.U. after 1 cycles

Zero-point correction= 0.117421
(Hartree/Particle)
Thermal correction to Energy= 0.123067
Thermal correction to Enthalpy= 0.124011
Thermal correction to Gibbs Free Energy= 0.088272
Sum of electronic and zero-point Energies= -270.549228
Sum of electronic and thermal Energies= -270.543583
Sum of electronic and thermal Enthalpies= -270.542638
Sum of electronic and thermal Free Energies= -270.578378

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.226	22.070	75.220

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

1	6	0	0.000040	-1.122467	1.236221
2	6	0	-0.000041	-1.804513	-0.000000
3	6	0	0.000040	-1.122467	-1.236221
4	6	0	0.000040	0.254593	-1.246704
5	6	0	0.000032	0.983959	0.000000
6	6	0	0.000040	0.254593	1.246704
7	1	0	0.000066	-1.684936	2.164267
8	1	0	-0.000215	-2.891872	-0.000000
9	1	0	0.000007	0.807271	-2.182219
10	1	0	0.000007	0.807271	2.182219
11	1	0	0.000066	-1.684936	-2.164267
12	6	0	-0.000090	2.355744	0.000000
13	1	0	-0.000153	2.925277	-0.926996
14	1	0	-0.000153	2.925277	0.926996

benzene.log

SCF Done: E(RB3LYP) = -232.258922022 A.U. after 1 cycles

Zero-point correction= 0.100550
(Hartree/Particle)
Thermal correction to Energy= 0.104947
Thermal correction to Enthalpy= 0.105891
Thermal correction to Gibbs Free Energy= 0.073079
Sum of electronic and zero-point Energies= -232.158372
Sum of electronic and thermal Energies= -232.153975
Sum of electronic and thermal Enthalpies= -232.153031
Sum of electronic and thermal Free Energies= -232.185843

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	65.855	17.168	69.059

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.255077	0.617277	0.000000
2	6	0	-1.162116	-0.778283	0.000000
3	6	0	0.092957	-1.395552	-0.000000
4	6	0	1.255077	-0.617277	-0.000000
5	6	0	1.162116	0.778283	-0.000000
6	6	0	-0.092957	1.395552	0.000000
7	1	0	-2.230858	1.097193	-0.000001
8	1	0	-2.065622	-1.383384	-0.000000

9	1	0	2.230858	-1.097193	0.000000
10	1	0	2.065622	1.383384	0.000000
11	1	0	-0.165229	2.480561	-0.000000
12	1	0	0.165229	-2.480561	-0.000000

o-tolCH2+.log

SCF Done: E(RB3LYP) = -309.990897173 A.U. after 1 cycles

Zero-point correction= 0.145086
(Hartree/Particle)
Thermal correction to Energy= 0.152399
Thermal correction to Enthalpy= 0.153343
Thermal correction to Gibbs Free Energy= 0.113677
Sum of electronic and zero-point Energies= -309.845811
Sum of electronic and thermal Energies= -309.838498
Sum of electronic and thermal Enthalpies= -309.837554
Sum of electronic and thermal Free Energies= -309.877221

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	95.632	28.046	83.485

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.715761	-1.010720	-0.000191
2	6	0	0.389335	-1.474083	-0.000307
3	6	0	-0.681934	-0.592116	0.000012
4	6	0	-0.371017	0.837336	0.000139
5	6	0	1.010419	1.276891	0.000312
6	6	0	2.035837	0.365681	0.000136
7	1	0	2.522680	-1.739727	-0.000310
8	1	0	0.204244	-2.543878	-0.000540
9	1	0	1.212869	2.344469	0.000536
10	1	0	3.072363	0.686183	0.000229
11	6	0	-2.094267	-1.098911	0.000330
12	1	0	-2.644913	-0.755928	0.885101
13	1	0	-2.645337	-0.756347	-0.884361
14	1	0	-2.112338	-2.190823	0.000504
15	6	0	-1.353075	1.790258	-0.000398
16	1	0	-1.105655	2.849290	-0.000531
17	1	0	-2.410270	1.540747	-0.000833

m-tolCH2+.log

```
 SCF Done:  E(RB3LYP) =  -309.990257688     A.U. after    1 cycles


 Zero-point correction=                           0.144934
(Hartree/Particle)
 Thermal correction to Energy=                    0.152338
 Thermal correction to Enthalpy=                  0.153282
 Thermal correction to Gibbs Free Energy=         0.113330
 Sum of electronic and zero-point Energies=           -309.845324
 Sum of electronic and thermal Energies=              -309.837920
 Sum of electronic and thermal Enthalpies=            -309.836975
 Sum of electronic and thermal Free Energies=         -309.876928

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  95.594             28.163             84.086


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.258948   -0.410608   -0.000041
      2          6           0       -0.053389   -1.012099   -0.000032
      3          6           0       -1.196707   -0.235415   -0.000022
      4          6           0       -1.018900    1.173936    0.000052
      5          6           0        0.244026    1.800520    0.000025
      6          6           0        1.382835    1.026753   -0.000068
      7          1           0       -0.125644   -2.096836    0.000009
      8          1           0       -1.906707    1.803700    0.000125
      9          1           0        0.307073    2.883986    0.000081
     10          1           0        2.371402    1.477124   -0.000193
     11          6           0       -2.582533   -0.827589   -0.000011
     12          1           0       -3.144768   -0.503935    0.883655
     13          1           0       -3.145253   -0.502820   -0.882959
     14          1           0       -2.551500   -1.920108   -0.000718
     15          6           0        2.382111   -1.197613    0.000074
     16          1           0        2.316893   -2.283549    0.000101
     17          1           0        3.380162   -0.764885    0.000036
 ---------------------------------------------------------------------
```

p-tolCH2+.log

```
 SCF Done:  E(RB3LYP) =  -309.996515845     A.U. after    8 cycles
```

```
 Zero-point correction=                           0.144644
(Hartree/Particle)
 Thermal correction to Energy=                    0.152141
 Thermal correction to Enthalpy=                  0.153085
 Thermal correction to Gibbs Free Energy=         0.112247
 Sum of electronic and zero-point Energies=           -309.851872
 Sum of electronic and thermal Energies=              -309.844375
 Sum of electronic and thermal Enthalpies=            -309.843430
 Sum of electronic and thermal Free Energies=         -309.884269

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  95.470             28.118             85.951


 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.487529   -0.000001    0.001684
      2          6           0       -0.748857   -1.242062   -0.002274
      3          6           0        0.622569   -1.230905   -0.010977
      4          6           0        1.337804    0.000002   -0.013971
      5          6           0        0.622567    1.230907   -0.010976
      6          6           0       -0.748859    1.242062   -0.002274
      7          1           0       -1.296371   -2.180721   -0.000793
      8          1           0        1.177739    2.164186   -0.017470
      9          1           0       -1.296375    2.180720   -0.000794
     10          6           0       -2.856056   -0.000002    0.009861
     11          1           0       -3.425344   -0.926753    0.013682
     12          1           0       -3.425345    0.926750    0.013681
     13          6           0        2.829159    0.000000    0.008342
     14          1           0        3.169439   -0.000067    1.057074
     15          1           0        3.246866   -0.894731   -0.462252
     16          1           0        3.246871    0.894783   -0.462146
     17          1           0        1.177743   -2.164182   -0.017470
 ---------------------------------------------------------------------
```

o-CH3Ph2CH+.log

```
 SCF Done:  E(RB3LYP) =  -541.083946233     A.U. after    1 cycles


 Zero-point correction=                           0.227436
(Hartree/Particle)
 Thermal correction to Energy=                    0.239069
 Thermal correction to Enthalpy=                  0.240013
 Thermal correction to Gibbs Free Energy=         0.189196
```

```
Sum of electronic and zero-point Energies=          -540.856511
Sum of electronic and thermal Energies=             -540.844877
Sum of electronic and thermal Enthalpies=           -540.843933
Sum of electronic and thermal Free Energies=        -540.894751

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  150.018             46.176            106.955
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.411544	-1.943053	0.391149
2	6	0	1.199617	-1.281891	0.398762
3	6	0	1.121709	0.119190	0.118854
4	6	0	2.336806	0.858119	-0.133159
5	6	0	3.537523	0.151166	-0.155848
6	6	0	3.582314	-1.224427	0.097213
7	1	0	2.462967	-2.999953	0.632704
8	1	0	0.303116	-1.813451	0.696090
9	1	0	4.461008	0.681800	-0.367968
10	1	0	4.540607	-1.736745	0.087569
11	6	0	-0.111274	0.811095	0.147669
12	1	0	-0.039456	1.888514	0.286532
13	6	0	-1.444914	0.333001	0.030314
14	6	0	-2.488059	1.193847	0.484577
15	6	0	-1.800078	-0.919405	-0.551903
16	6	0	-3.812102	0.787434	0.438052
17	1	0	-2.231254	2.165477	0.898508
18	6	0	-3.129010	-1.304051	-0.619626
19	1	0	-1.037288	-1.543468	-1.003554
20	6	0	-4.133121	-0.462768	-0.110920
21	1	0	-4.597249	1.438349	0.809624
22	1	0	-3.397948	-2.247605	-1.084372
23	1	0	-5.172621	-0.773700	-0.168053
24	6	0	2.339771	2.339007	-0.419399
25	1	0	1.780189	2.582819	-1.330046
26	1	0	1.901106	2.916299	0.404682
27	1	0	3.362476	2.698081	-0.556128

m-CH3Ph2CH+.log

```
SCF Done:  E(RB3LYP) =  -541.086037911     A.U. after    1 cycles
```

Zero-point correction=	0.227118
(Hartree/Particle)	
Thermal correction to Energy=	0.238967
Thermal correction to Enthalpy=	0.239912
Thermal correction to Gibbs Free Energy=	0.188147
Sum of electronic and zero-point Energies=	-540.858920
Sum of electronic and thermal Energies=	-540.847071
Sum of electronic and thermal Enthalpies=	-540.846126
Sum of electronic and thermal Free Energies=	-540.897891

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.954	46.365	108.947

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.273260	-1.800078	0.427559
2	6	0	1.019427	-1.213628	0.424208
3	6	0	0.894821	0.176413	0.134719
4	6	0	2.080734	0.939023	-0.095749
5	6	0	3.339765	0.351158	-0.121278
6	6	0	3.413541	-1.032505	0.142992
7	1	0	2.381066	-2.852856	0.670025
8	1	0	0.150871	-1.795310	0.708857
9	1	0	4.388356	-1.515101	0.151749
10	6	0	-0.335698	0.877429	0.097398
11	1	0	-0.236811	1.961653	0.161651
12	6	0	-1.675543	0.420225	-0.008370
13	6	0	-2.705019	1.346500	0.336793
14	6	0	-2.051736	-0.876171	-0.468803
15	6	0	-4.038053	0.969468	0.301698
16	1	0	-2.430894	2.347868	0.658259
17	6	0	-3.388120	-1.234056	-0.525135
18	1	0	-1.298054	-1.561486	-0.838531
19	6	0	-4.380150	-0.321588	-0.125903
20	1	0	-4.813094	1.672871	0.589254
21	1	0	-3.672604	-2.213551	-0.896916
22	1	0	-5.425907	-0.612529	-0.173546
23	6	0	4.588580	1.148902	-0.404540
24	1	0	4.368917	2.214594	-0.513328
25	1	0	5.320035	1.034003	0.403506
26	1	0	5.068387	0.807623	-1.329573
27	1	0	1.984882	2.005666	-0.284949

p-CH3Ph2CH+.log

SCF Done: E(RB3LYP) = -541.089569583 A.U. after 1 cycles

Zero-point correction= 0.226915
(Hartree/Particle)
Thermal correction to Energy= 0.238868
Thermal correction to Enthalpy= 0.239813
Thermal correction to Gibbs Free Energy= 0.186578
Sum of electronic and zero-point Energies= -540.862654
Sum of electronic and thermal Energies= -540.850701
Sum of electronic and thermal Enthalpies= -540.849757
Sum of electronic and thermal Free Energies= -540.902992

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	149.892	46.343	112.042

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.479399	1.166690	0.370840
2	6	0	-1.157458	0.775467	0.368871
3	6	0	-0.799482	-0.563981	0.020467
4	6	0	-1.855626	-1.481724	-0.268957
5	6	0	-3.174308	-1.068542	-0.287814
6	6	0	-3.515809	0.263082	0.027058
7	1	0	-2.738222	2.181661	0.660433
8	1	0	-0.396296	1.473967	0.695930
9	6	0	0.520497	-1.063541	-0.023864
10	1	0	0.586689	-2.151947	-0.041301
11	6	0	1.781422	-0.405128	-0.045951
12	6	0	2.926415	-1.191555	0.276466
13	6	0	1.973626	0.960918	-0.403188
14	6	0	4.189756	-0.621990	0.317378
15	1	0	2.796104	-2.242843	0.519545
16	6	0	3.243352	1.514212	-0.384915
17	1	0	1.138014	1.554806	-0.754440
18	6	0	4.348831	0.731817	-0.009852
19	1	0	5.051877	-1.223853	0.587055
20	1	0	3.388234	2.549126	-0.679203
21	1	0	5.340466	1.175587	0.002428
22	1	0	-1.609115	-2.513361	-0.506536
23	1	0	-3.959103	-1.777358	-0.535027
24	6	0	-4.944230	0.719385	0.032530
25	1	0	-5.632325	-0.079751	-0.252995
26	1	0	-5.229416	1.082490	1.028646
27	1	0	-5.082426	1.560815	-0.658954

C6F5H.log

SCF Done: E(RB3LYP) = -728.432149873 A.U. after 1 cycles

Zero-point correction= 0.059666
(Hartree/Particle)
Thermal correction to Energy= 0.068339
Thermal correction to Enthalpy= 0.069283
Thermal correction to Gibbs Free Energy= 0.025755
Sum of electronic and zero-point Energies= -728.372484
Sum of electronic and thermal Energies= -728.363811
Sum of electronic and thermal Enthalpies= -728.362866
Sum of electronic and thermal Free Energies= -728.406395

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	42.883	32.079	91.613

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.209735	0.425213	0.000024
2	6	0	-1.194163	-0.968250	0.000050
3	6	0	-0.000020	-1.679282	0.000003
4	6	0	1.194166	-0.968255	0.000020
5	6	0	1.209751	0.425170	0.000036
6	6	0	-0.000001	1.119302	0.000003
7	1	0	0.000008	-2.763280	-0.000030
8	9	0	2.366941	-1.626734	-0.000026
9	9	0	2.367449	1.100325	-0.000005
10	9	0	0.000054	2.457178	-0.000020
11	9	0	-2.367461	1.100312	-0.000011
12	9	0	-2.366983	-1.626649	-0.000026

o-CH3Ph2CHF5+.log

SCF Done: E(RB3LYP) = -1037.23124015 A.U. after 1 cycles

Zero-point correction= 0.186002
(Hartree/Particle)
Thermal correction to Energy= 0.202191
Thermal correction to Enthalpy= 0.203135

Thermal correction to Gibbs Free Energy= 0.141734
Sum of electronic and zero-point Energies= -1037.045238
Sum of electronic and thermal Energies= -1037.029050
Sum of electronic and thermal Enthalpies= -1037.028105
Sum of electronic and thermal Free Energies= -1037.089506

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.876	61.111	129.228

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.256674	1.314191	0.284840
2	6	0	-0.909108	0.993847	0.290354
3	6	0	-0.447437	-0.326085	0.023719
4	6	0	-1.458635	-1.304334	-0.215033
5	6	0	-2.807359	-0.995908	-0.249974
6	6	0	-3.207826	0.322853	0.001529
7	6	0	0.902672	-0.789528	0.093701
8	1	0	0.964912	-1.855198	0.297563
9	6	0	2.135490	-0.139302	-0.073737
10	6	0	3.341091	-0.826756	0.354558
11	6	0	2.249130	1.122921	-0.746945
12	6	0	4.562150	-0.197327	0.132362
13	6	0	3.479719	1.697210	-0.973418
14	1	0	1.359502	1.604150	-1.132174
15	6	0	4.638357	1.040679	-0.517227
16	1	0	5.476692	-0.678966	0.464739
17	1	0	3.557709	2.639327	-1.506190
18	1	0	5.612096	1.494011	-0.683204
19	9	0	-1.093460	-2.563878	-0.453147
20	9	0	-3.715902	-1.926550	-0.512452
21	9	0	-4.486821	0.633638	-0.016790
22	9	0	-2.658888	2.547985	0.565672
23	9	0	-0.053284	1.953613	0.642271
24	6	0	3.308673	-2.157512	1.060367
25	1	0	2.761222	-2.106113	2.008739
26	1	0	2.838018	-2.936356	0.446150
27	1	0	4.323588	-2.493820	1.283827

m-CH3Ph2CHF5+.log

SCF Done: E(RB3LYP) = -1037.23314125 A.U. after 9 cycles

Zero-point correction= 0.185814
(Hartree/Particle)
Thermal correction to Energy= 0.202187
Thermal correction to Enthalpy= 0.203132
Thermal correction to Gibbs Free Energy= 0.140815
Sum of electronic and zero-point Energies= -1037.047327
Sum of electronic and thermal Energies= -1037.030954
Sum of electronic and thermal Enthalpies= -1037.030010
Sum of electronic and thermal Free Energies= -1037.092326

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.875	61.247	131.156

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.463945	1.265920	0.201544
2	6	0	-1.109343	0.980502	0.205416
3	6	0	-0.614847	-0.344705	0.039811
4	6	0	-1.606876	-1.364669	-0.099024
5	6	0	-2.963543	-1.093539	-0.128643
6	6	0	-3.394138	0.230850	0.022822
7	6	0	0.743507	-0.776293	0.099854
8	1	0	0.827415	-1.839732	0.315694
9	6	0	1.985579	-0.136313	-0.076827
10	6	0	3.138462	-0.901969	0.305899
11	6	0	2.184517	1.150726	-0.666593
12	6	0	4.427750	-0.406987	0.179470
13	6	0	3.468840	1.633638	-0.825964
14	1	0	1.345390	1.730902	-1.024450
15	6	0	4.571185	0.875288	-0.395051
16	1	0	3.631526	2.601089	-1.290579
17	1	0	5.571311	1.283439	-0.524308
18	9	0	-1.218068	-2.630514	-0.242226
19	9	0	-3.851956	-2.064826	-0.293611
20	9	0	-4.680347	0.507275	0.006723
21	9	0	-2.893088	2.508814	0.384174
22	9	0	-0.274471	1.990149	0.448505
23	6	0	5.637258	-1.194863	0.616512
24	1	0	6.169324	-0.676208	1.422798
25	1	0	5.360179	-2.187987	0.980360
26	1	0	6.343498	-1.321407	-0.211950
27	1	0	2.986288	-1.893689	0.725008

p-CH3Ph2CHF5+.log

SCF Done: E(RB3LYP) = -1037.23774487 A.U. after 1 cycles

Zero-point correction= 0.185562
(Hartree/Particle)
Thermal correction to Energy= 0.202037
Thermal correction to Enthalpy= 0.202982
Thermal correction to Gibbs Free Energy= 0.139366
Sum of electronic and zero-point Energies= -1037.052183
Sum of electronic and thermal Energies= -1037.035707
Sum of electronic and thermal Enthalpies= -1037.034763
Sum of electronic and thermal Free Energies= -1037.098379

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	126.780	61.232	133.890

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.346553	1.390130	0.133596
2	6	0	-1.037847	0.944659	0.214904
3	6	0	-0.699506	-0.432712	0.109128
4	6	0	-1.797803	-1.330141	-0.053920
5	6	0	-3.109599	-0.900596	-0.159669
6	6	0	-3.385150	0.469074	-0.065423
7	6	0	0.596478	-1.020130	0.248731
8	1	0	0.543468	-2.075395	0.509490
9	6	0	1.906859	-0.539457	0.101525
10	6	0	2.952939	-1.421747	0.538072
11	6	0	2.293016	0.701348	-0.504638
12	6	0	4.279536	-1.061871	0.437114
13	6	0	3.622934	1.031437	-0.625534
14	1	0	1.543974	1.370738	-0.904959
15	6	0	4.646225	0.173014	-0.143787
16	1	0	3.901084	1.965926	-1.104917
17	9	0	-1.557692	-2.638060	-0.144400
18	9	0	-4.099083	-1.765374	-0.344862
19	9	0	-4.627518	0.896230	-0.154864
20	9	0	-2.629386	2.681513	0.261261
21	9	0	-0.098473	1.855415	0.474918
22	1	0	2.685507	-2.381741	0.971740
23	1	0	5.052738	-1.736112	0.792952
24	6	0	6.081961	0.576938	-0.264249
25	1	0	6.280023	1.453375	0.369308
26	1	0	6.763540	-0.222391	0.035269
27	1	0	6.318089	0.878407	-1.292462

3+_smd(CH2Cl2).log

SCF Done: E(RB3LYP) = -644.945666885 A.U. after 7 cycles

Zero-point correction= 0.283235
(Hartree/Particle)
Thermal correction to Energy= 0.298598
Thermal correction to Enthalpy= 0.299543
Thermal correction to Gibbs Free Energy= 0.241488
Sum of electronic and zero-point Energies= -644.662432
Sum of electronic and thermal Energies= -644.647068
Sum of electronic and thermal Enthalpies= -644.646124
Sum of electronic and thermal Free Energies= -644.704179

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.373	54.777	122.186

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.138590	-0.134962	-0.068909
2	6	0	0.269293	1.666279	0.247279
3	1	0	-0.686313	2.139684	0.509959
4	6	0	1.236798	1.805371	1.448685
5	1	0	2.214095	1.359243	1.234267
6	1	0	1.394052	2.872778	1.650307
7	1	0	0.842258	1.352181	2.365907
8	6	0	1.156829	-1.447961	-0.374698
9	1	0	0.679837	-2.158766	-1.066364
10	6	0	1.356688	-2.189142	0.982381
11	1	0	2.014864	-3.049761	0.808961
12	1	0	1.838702	-1.548803	1.730140
13	1	0	0.420918	-2.575001	1.405321
14	6	0	-1.924295	-0.690176	-0.031583
15	1	0	-1.909905	-1.787144	0.017680
16	6	0	-2.721408	-0.135401	1.166274
17	1	0	-3.753416	-0.504729	1.110818
18	1	0	-2.305003	-0.455086	2.128415
19	1	0	-2.760808	0.960135	1.156432
20	6	0	2.493441	-0.976815	-0.971000
21	1	0	3.000642	-0.259885	-0.316329
22	1	0	3.157432	-1.841984	-1.093805
23	1	0	2.364326	-0.514047	-1.955287
24	6	0	0.829395	2.368536	-1.014216
25	1	0	0.140783	2.319650	-1.865740
26	1	0	0.988255	3.428930	-0.779562

27	1	0	1.791996	1.948064	-1.322950
28	6	0	-2.568804	-0.276695	-1.384912
29	1	0	-2.051410	-0.704820	-2.252276
30	1	0	-3.601616	-0.647473	-1.404933
31	1	0	-2.607047	0.812313	-1.505491

4+_smd(CH2Cl2).log

SCF Done: E(RB3LYP) = -527.008943516 A.U. after 8 cycles

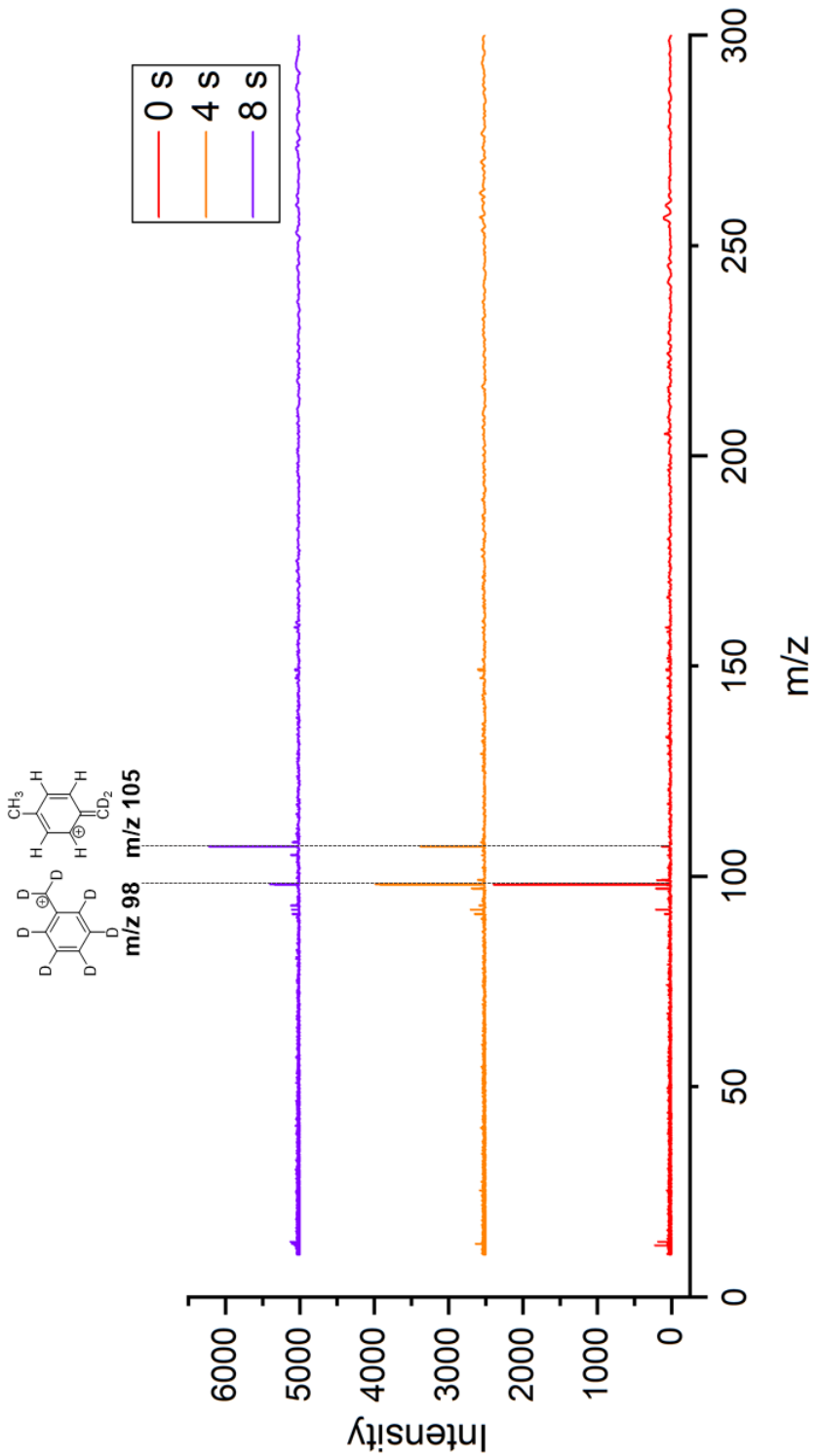
Zero-point correction= 0.197574
(Hartree/Particle)
Thermal correction to Energy= 0.208940
Thermal correction to Enthalpy= 0.209884
Thermal correction to Gibbs Free Energy= 0.159851
Sum of electronic and zero-point Energies= -526.811369
Sum of electronic and thermal Energies= -526.800004
Sum of electronic and thermal Enthalpies= -526.799060
Sum of electronic and thermal Free Energies= -526.849092

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	131.112	38.743	105.302

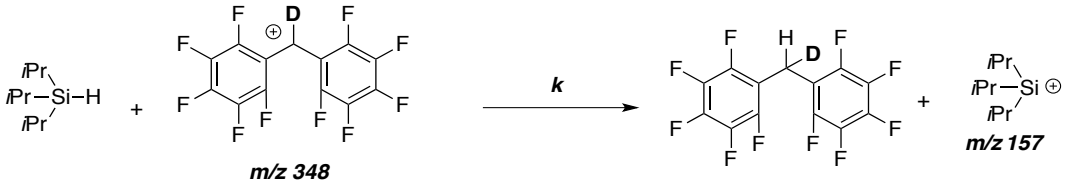
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.095507	-0.077701	-0.271742
2	6	0	0.150224	1.716208	0.124710
3	1	0	-0.527958	2.271329	-0.544413
4	1	0	-0.283205	1.862421	1.128825
5	6	0	1.581989	2.271614	0.051570
6	1	0	1.998364	2.184372	-0.957527
7	1	0	1.578660	3.333964	0.319739
8	1	0	2.253873	1.755429	0.745265
9	6	0	1.325898	-1.220485	-0.609227
10	1	0	0.997587	-1.973127	-1.337641
11	1	0	2.152332	-0.655964	-1.056332
12	6	0	1.805709	-1.926217	0.691607
13	1	0	2.630008	-2.602087	0.439128
14	1	0	2.176560	-1.212505	1.434814
15	1	0	1.012555	-2.525650	1.151436
16	6	0	-1.810535	-0.780279	-0.289968
17	1	0	-2.034237	-0.942226	-1.360386
18	1	0	-1.749825	-1.794547	0.132656
19	6	0	-2.923511	0.045930	0.376863

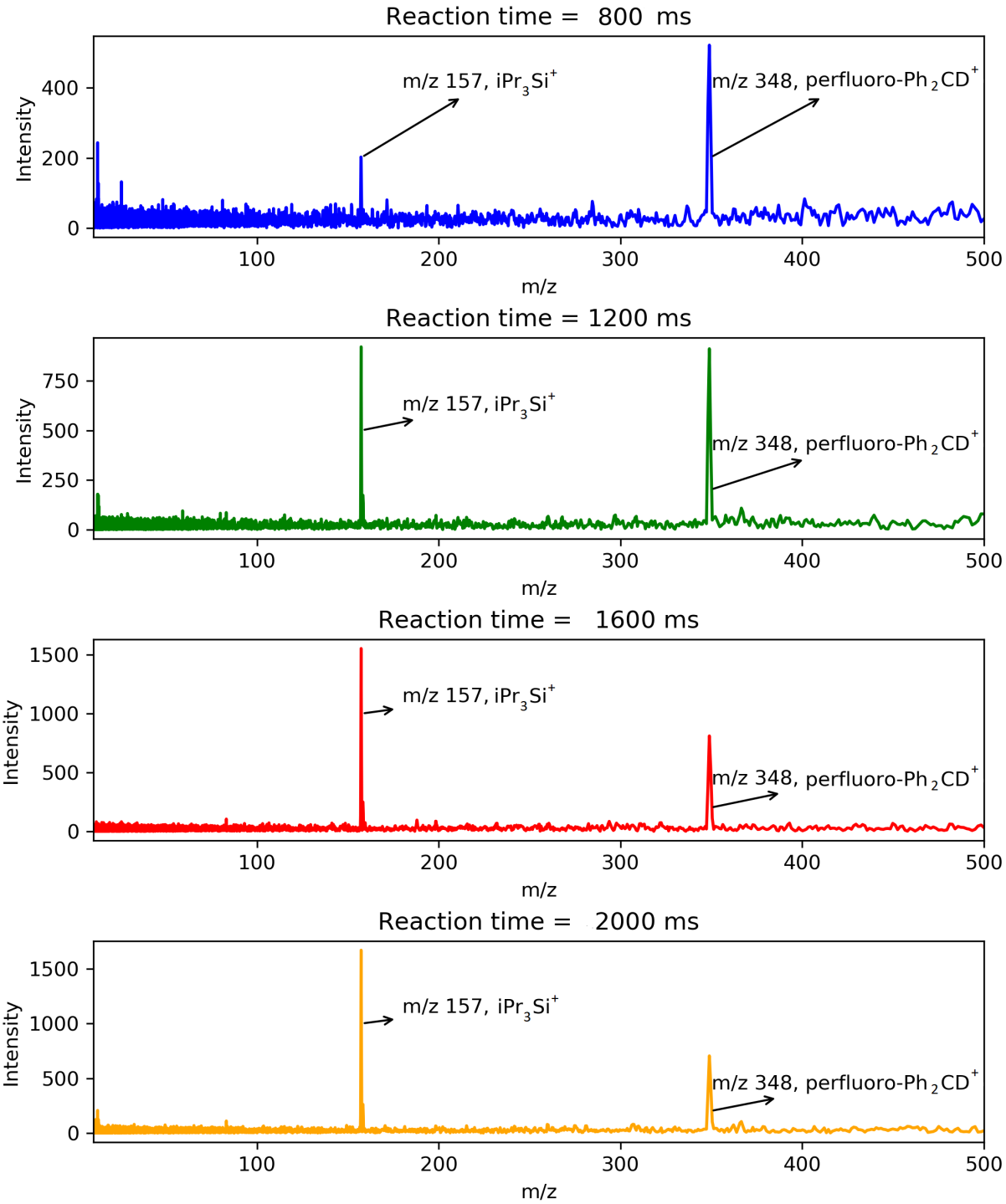
20	1	0	-3.885563	-0.463493	0.252957
21	1	0	-2.745900	0.167064	1.451043
22	1	0	-3.014796	1.042204	-0.068498

Spectra example for reaction: $C_6D_5CD_2^+$ and toluene



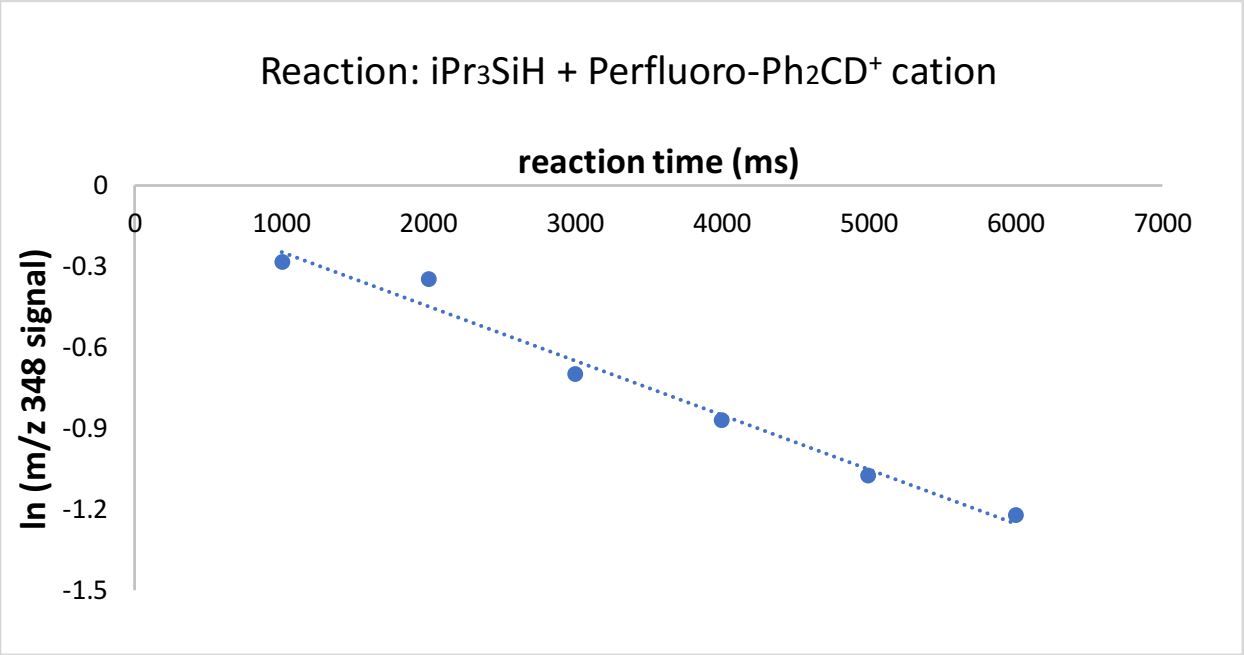
Spectra example #1: reaction between 3 and 1a-D:



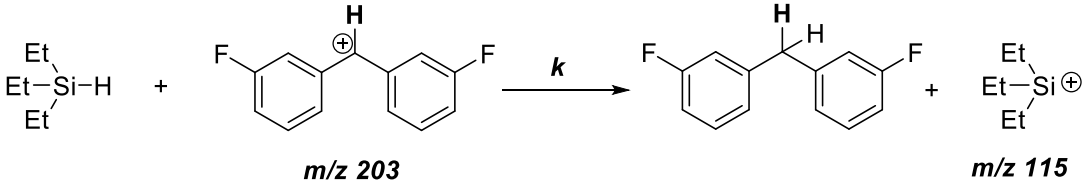


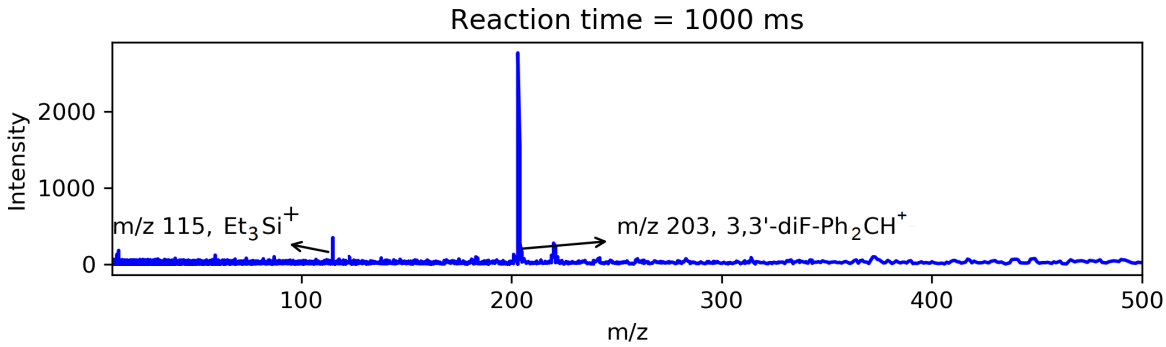
Plot of the kinetics #1: reaction between 3 and 1a-D:

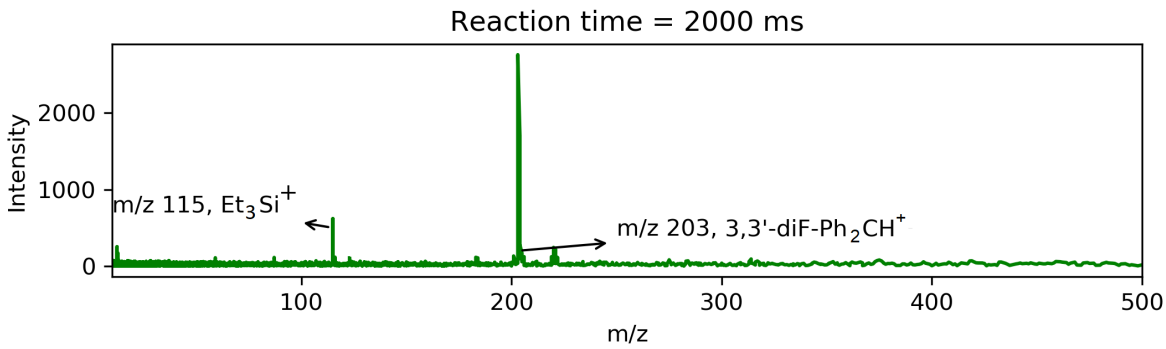
The pressure of 3 is the average of pre-pressure and post-pressure.

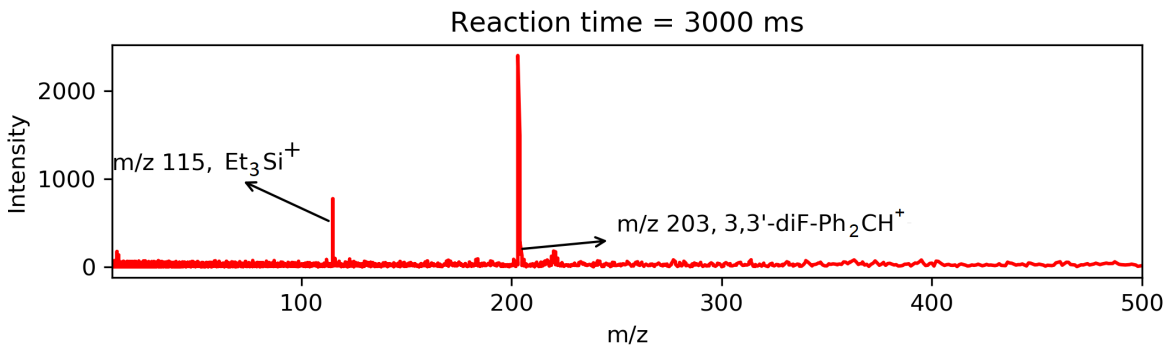


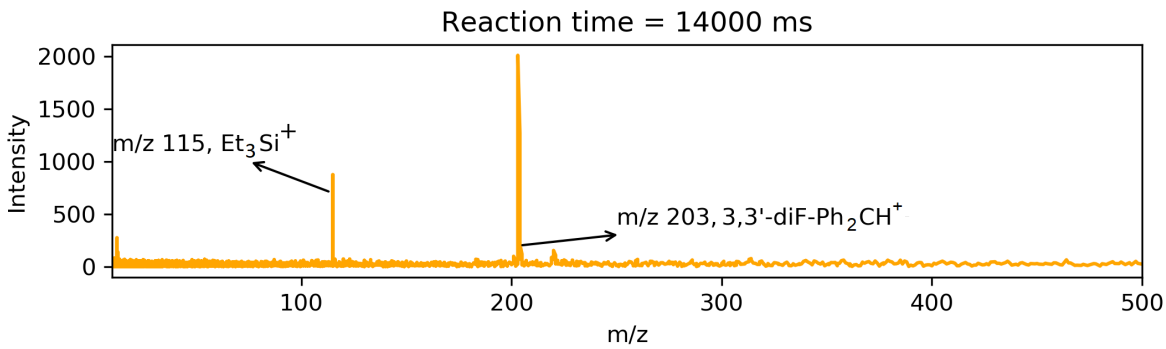
Spectra example #2: reaction between 4 and 1c:











Plot of the kinetics #2: reaction between 4 and 1c:

The pressure of 4 is the average of pre-pressure and post-pressure.