Supporting Information for:

A Joint Experimental and Theoretical Study of the Palladium Catalyzed Electrophilic Allylation of Aldehydes

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Experimental Section

General remarks

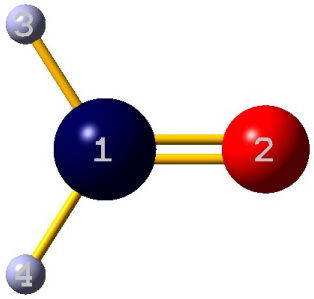
All reactions were performed under an inert atmosphere of argon or nitrogen by using Schlenk and glove-box techniques and dry deoxygenated solvents. Dry THF, ether and hexanes were obtained by distillation from Na/benzophenone. Dry dichloromethane was distilled on P_2O_5 and dry toluene on Na. Nuclear magnetic resonance spectra were recorded on a spectrometer operating at 300.0 MHz for ^{1}H. Solvent peaks are used as internal reference relative to Me_4Si. Complexes **1** and **2** were prepared according to literature procedures (Doux, M.; Mezailles, N.; Melaimi, M.; Ricard, L.; Le Floch, P. *Chem. Commun.* **2002**, 1566-1567, Chentit, M., *PhD Thesis*, Faculté des sciences de l'Université de Genève: Geneva, **1999**).

DFT Data

I. Non catalysed reaction

With formaldehyde

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **formaldehyde**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.005969
2	8	0	0.000000	0.000000	1.210723
3	1	0	0.938640	0.000000	-0.586832
4	1	0	-0.938640	0.000000	-0.586832

HF= -114.4539699

	1	2	3
	B2	?A	B2
Frequencies --	1196.3616	1278.7960	1560.0286
Red. masses --	1.3698	1.3421	1.1157
Frc consts --	1.1551	1.2931	1.5998
IR Inten --	2.0612	11.7910	5.5458

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.17	0.00	0.15	0.00	0.00	0.00	0.00	-0.01
2	8	0.00	-0.04	0.00	-0.08	0.00	0.00	0.00	0.00	0.08
3	1	0.00	-0.70	0.00	-0.25	0.00	-0.65	-0.35	0.00	-0.61
4	1	0.00	-0.70	0.00	-0.25	0.00	0.65	0.35	0.00	-0.61

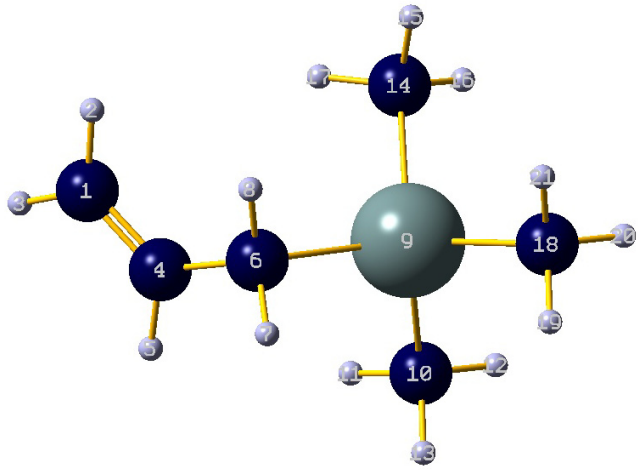
thermodynamics:
Sum of electronic and zero-point Energies= -114.427067

Sum of electronic and thermal Enthalpies= -114.423256

Sum of electronic and thermal Free Energies= -114.448074

Total free energy in solution:
with all non electrostatic terms (a.u.) = -114.453337

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **allyltrimethyltin**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.022835	-0.227431	-0.071966
2	1	0	-0.008109	-0.425527	0.998579
3	1	0	0.935291	-0.242183	-0.584479
4	6	0	-1.162675	0.029218	-0.724195
5	1	0	-1.108143	0.224357	-1.797434
6	6	0	-2.530785	0.037645	-0.136258
7	1	0	-3.121108	0.885753	-0.504809
8	1	0	-2.496426	0.102689	0.957719
9	50	0	-3.615828	-1.789277	-0.654445
10	6	0	-3.607756	-2.030743	-2.796827
11	1	0	-2.583208	-2.104194	-3.175398
12	1	0	-4.143006	-2.942309	-3.082814
13	1	0	-4.095444	-1.181827	-3.287355
14	6	0	-2.613607	-3.447510	0.283503
15	1	0	-2.796229	-3.453795	1.362971
16	1	0	-2.960005	-4.400663	-0.128984
17	1	0	-1.534486	-3.369591	0.117422
18	6	0	-5.650306	-1.635792	0.048116
19	1	0	-6.150979	-0.771849	-0.401193
20	1	0	-6.218148	-2.534338	-0.215716
21	1	0	-5.679699	-1.520747	1.136566

HF=-240.3469727

	1	2	3
	A	A	A
Frequencies --	35.0426	62.8355	73.3317

Red. masses --		2.7468			2.0389			1.1667		
Frc consts --		0.0020			0.0047			0.0037		
IR Inten --		0.0844			0.2089			0.0443		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.01	0.24	0.05	0.22	0.03	0.02	0.07	0.02
2	1	-0.17	0.16	0.27	0.07	0.31	0.04	0.03	0.10	0.02
3	1	0.05	-0.08	0.37	0.06	0.27	0.03	0.03	0.09	0.02
4	6	0.07	-0.07	0.05	0.03	0.04	0.00	0.02	0.01	0.00
5	1	0.22	-0.22	0.02	0.01	-0.05	-0.01	0.01	-0.02	0.00
6	6	-0.01	0.04	-0.14	0.03	-0.04	0.00	0.01	-0.02	0.00
7	1	0.06	0.00	-0.32	0.00	-0.05	0.01	0.01	-0.02	0.00
8	1	-0.15	0.18	-0.14	0.03	-0.03	0.00	0.01	-0.02	0.00
9	50	0.00	0.00	-0.02	0.00	-0.02	0.00	0.00	-0.01	0.00
10	6	-0.17	-0.06	-0.02	-0.03	-0.01	0.00	-0.01	-0.01	0.00
11	1	-0.20	-0.10	-0.10	-0.05	-0.41	0.02	0.00	0.53	-0.07
12	1	-0.21	-0.06	0.05	-0.38	0.20	-0.02	0.45	-0.28	0.03
13	1	-0.19	-0.07	-0.01	0.31	0.18	-0.01	-0.48	-0.26	0.03
14	6	0.10	0.05	-0.05	-0.10	-0.11	-0.03	-0.05	-0.04	-0.01
15	1	0.12	0.04	-0.05	0.00	-0.04	-0.01	0.06	0.04	0.01
16	1	0.14	0.03	-0.05	-0.28	-0.08	0.04	-0.18	-0.03	0.08
17	1	0.09	0.11	-0.07	-0.11	-0.26	-0.14	-0.06	-0.16	-0.12
18	6	0.05	0.00	0.12	0.02	0.09	0.01	0.01	0.05	0.01
19	1	0.02	0.01	0.18	0.08	0.14	0.03	0.04	0.08	0.04
20	1	0.03	0.00	0.15	-0.05	0.14	-0.01	-0.03	0.08	-0.01
21	1	0.13	-0.02	0.13	0.03	0.07	0.01	0.02	0.02	0.01

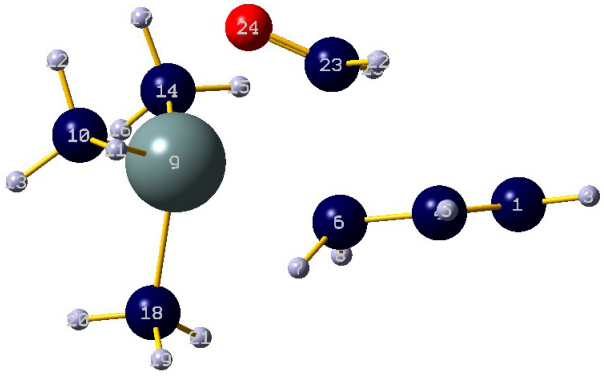
thermodynamics:
Sum of electronic and zero-point Energies= -240.168105

Sum of electronic and thermal Enthalpies= -240.154175

Sum of electronic and thermal Free Energies= -240.209027

Total free energy in solution:
with all non electrostatic terms (a.u.) = -240.330308

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS$_\alpha$**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.988629	0.399040	0.397987
2	1	0	3.748419	0.682994	1.421359
3	1	0	5.026545	0.154173	0.190272
4	6	0	3.057213	0.382517	-0.565346
5	1	0	3.358303	0.098348	-1.575277
6	6	0	1.615708	0.667376	-0.375589
7	1	0	1.225872	1.157739	-1.277085
8	1	0	1.490357	1.337641	0.483014
9	50	0	-0.817994	0.084277	0.026408
10	6	0	-1.857247	-0.604990	-1.714433
11	1	0	-1.169783	-0.635509	-2.565353

12	1	0	-2.236921	-1.615477	-1.547319
13	1	0	-2.681679	0.074356	-1.954363
14	6	0	-1.343230	-0.461282	2.032649
15	1	0	-0.451024	-0.448678	2.667538
16	1	0	-2.067931	0.247481	2.446159
17	1	0	-1.756669	-1.472667	2.046530
18	6	0	-1.058146	2.251838	-0.015301
19	1	0	-0.732615	2.690427	-0.963607
20	1	0	-2.129185	2.460083	0.105874
21	1	0	-0.523275	2.745586	0.802104
22	1	0	2.139405	-1.747804	-0.659856
23	6	0	1.345395	-1.478182	0.052220
24	8	0	0.178727	-1.955476	-0.108636
25	1	0	1.740141	-1.236646	1.055567

HF=-354.7388016

		1			2			3		
		A			A			A		
Frequencies --		-373.8099			40.1914			57.7503		
Red. masses --		6.7054			3.3422			2.1117		
Frc consts --		0.5521			0.0032			0.0041		
IR Inten --		70.7005			0.0738			0.1793		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.09	-0.02	-0.02	-0.05	-0.05	0.18	-0.09	0.14	0.09
2	1	-0.01	0.06	-0.02	-0.12	-0.13	0.19	-0.20	0.33	0.01
3	1	-0.11	-0.10	-0.06	-0.03	-0.03	0.23	-0.06	0.13	0.25
4	6	-0.15	-0.02	0.03	0.02	0.04	0.11	0.01	-0.07	0.00
5	1	-0.18	-0.08	0.03	0.09	0.12	0.11	0.12	-0.26	0.09
6	6	-0.13	0.32	-0.02	0.01	0.02	0.04	-0.01	-0.06	-0.19
7	1	0.09	0.50	-0.01	0.05	0.07	0.05	0.03	-0.28	-0.33
8	1	0.05	0.38	-0.04	-0.04	-0.03	0.07	-0.08	0.14	-0.36
9	50	0.04	0.05	-0.01	0.00	0.00	-0.01	0.01	0.00	0.00
10	6	0.05	-0.05	0.02	-0.19	-0.05	0.12	-0.04	0.04	0.02
11	1	0.01	-0.03	-0.01	-0.30	-0.03	0.03	-0.04	-0.03	0.02
12	1	0.02	-0.04	0.01	-0.13	-0.06	0.17	-0.10	0.06	0.04
13	1	0.05	-0.02	0.09	-0.24	-0.07	0.22	0.01	0.08	0.00
14	6	0.04	-0.04	-0.02	0.22	0.06	0.05	0.03	-0.03	0.00
15	1	0.00	-0.02	0.02	0.27	0.14	-0.03	0.04	-0.03	0.00
16	1	0.02	-0.02	-0.08	0.22	0.04	0.09	0.04	-0.03	0.02
17	1	0.01	-0.03	-0.01	0.27	0.04	0.14	0.03	-0.03	-0.01
18	6	-0.11	0.03	0.01	-0.02	-0.01	-0.12	0.05	0.01	0.07
19	1	-0.07	0.01	0.02	-0.09	-0.07	-0.18	0.24	0.06	0.16
20	1	-0.09	0.14	0.01	-0.02	-0.01	-0.07	0.04	0.02	-0.11
21	1	-0.07	0.00	0.00	0.03	0.06	-0.19	-0.09	-0.06	0.21
22	1	-0.01	-0.05	-0.01	-0.01	0.04	-0.14	0.04	-0.09	0.13
23	6	-0.05	-0.40	0.07	-0.01	-0.01	-0.11	-0.03	-0.02	0.03
24	8	0.05	-0.30	0.00	-0.01	0.00	-0.13	-0.02	-0.02	-0.04
25	1	-0.15	-0.01	0.01	0.00	-0.08	-0.10	-0.12	0.06	0.05

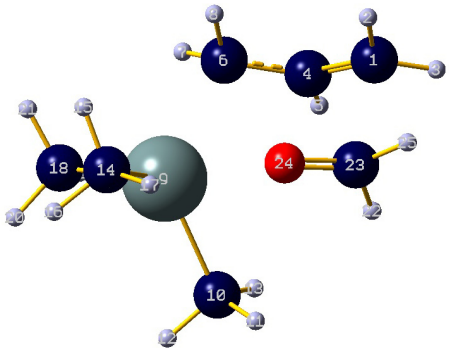
thermodynamics:
Sum of electronic and zero-point Energies= -354.529961

Sum of electronic and thermal Enthalpies= -354.513920

Sum of electronic and thermal Free Energies= -354.572813

Total free energy in solution:
with all non electrostatic terms (a.u.) = -354.724733

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for $\mathbf{TS}_{\gamma}$.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.171245	0.605570	-0.252747
2	1	0	-3.316010	0.307974	-1.288453
3	1	0	-4.061011	0.609214	0.372520
4	6	0	-2.091200	1.391860	0.078420
5	1	0	-2.084961	1.852116	1.068966
6	6	0	-0.892911	1.499975	-0.691351
7	1	0	-0.318039	2.409415	-0.509275
8	1	0	-1.007066	1.293127	-1.757892
9	50	0	0.714307	-0.029229	0.008213
10	6	0	0.586239	-0.717524	2.049946
11	1	0	0.159979	-1.722873	2.106012
12	1	0	1.591267	-0.734215	2.484904
13	1	0	-0.025227	-0.043654	2.660182
14	6	0	1.553128	-1.334864	-1.480098
15	1	0	1.537999	-0.848778	-2.461733
16	1	0	2.597170	-1.556000	-1.232989
17	1	0	0.985952	-2.265836	-1.541739
18	6	0	2.228959	1.546440	0.159939
19	1	0	1.952261	2.297569	0.909586
20	1	0	3.193854	1.116898	0.455858
21	1	0	2.370147	2.058056	-0.799485
22	1	0	-2.254887	-1.064036	1.358352
23	6	0	-2.265381	-1.236986	0.270503
24	8	0	-1.192930	-1.381873	-0.366875
25	1	0	-3.178836	-1.719363	-0.108122

HF=-354.7918743

	1			2			3		
	A			A			A		
Frequencies --	-269.9856			47.5780			64.7837		
Red. masses --	9.1326			1.1075			3.1852		
Frc consts --	0.3922			0.0015			0.0079		
IR Inten --	70.8448			0.0324			0.4204		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.27	0.48	-0.11	0.00	0.00	0.01	0.01	0.02	0.19
2 1	-0.14	0.09	-0.02	-0.01	-0.02	0.02	-0.11	0.13	0.17
3 1	-0.22	0.35	-0.05	0.01	0.02	0.02	0.07	-0.03	0.28
4 6	-0.07	-0.03	0.02	0.01	0.01	-0.02	0.05	-0.02	0.14
5 1	-0.01	-0.08	0.05	0.02	0.03	-0.03	0.16	-0.09	0.18
6 6	0.09	-0.22	0.05	0.00	-0.02	-0.04	-0.02	0.01	0.03
7 1	-0.07	-0.08	-0.07	0.00	-0.01	-0.07	0.00	0.00	0.01
8 1	-0.05	-0.07	0.03	-0.01	-0.05	-0.03	-0.12	0.05	0.04
9 50	0.03	0.06	-0.01	0.00	0.00	0.00	-0.01	0.00	-0.02
10 6	-0.04	-0.03	-0.03	0.01	-0.02	-0.01	-0.14	0.12	0.01
11 1	-0.02	-0.03	0.00	0.03	-0.02	-0.01	-0.24	0.17	0.07
12 1	-0.03	-0.02	-0.04	0.01	0.00	-0.01	-0.15	0.04	0.04
13 1	-0.03	-0.03	-0.02	0.00	-0.03	0.00	-0.07	0.23	-0.04
14 6	-0.03	-0.01	0.01	0.02	0.03	-0.02	0.12	-0.11	0.14
15 1	-0.02	-0.01	0.01	0.55	0.27	0.09	0.35	-0.13	0.13

16	1	-0.03	-0.01	0.01	-0.14	-0.40	0.30	0.05	-0.20	0.35
17	1	-0.01	-0.02	0.00	-0.28	0.24	-0.42	0.04	-0.06	0.06
18	6	0.09	-0.03	0.04	-0.02	0.01	0.03	0.00	0.00	-0.05
19	1	0.07	-0.02	0.02	-0.03	-0.01	0.04	0.00	0.03	-0.09
20	1	0.12	0.04	0.03	-0.01	0.02	0.03	0.00	0.00	-0.02
21	1	0.06	-0.03	0.03	-0.01	0.03	0.04	0.02	-0.04	-0.07
22	1	0.14	-0.02	0.04	0.01	0.03	0.04	0.06	-0.20	-0.08
23	6	0.09	-0.41	0.11	0.00	0.01	0.04	0.03	-0.06	-0.10
24	8	-0.12	-0.25	-0.03	-0.01	-0.01	0.03	0.01	0.02	-0.15
25	1	-0.16	0.10	0.07	-0.01	0.00	0.06	0.02	-0.01	-0.14

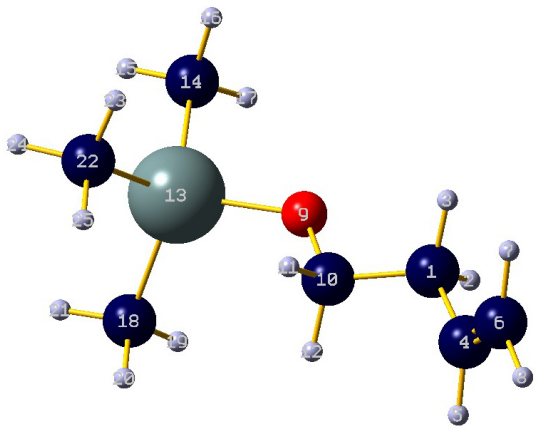
thermodynamics:
Sum of electronic and zero-point Energies= -354.581671

Sum of electronic and thermal Enthalpies= -354.566198

Sum of electronic and thermal Free Energies= -354.623274

Total free energy in solution:
with all non electrostatic terms (a.u.) = -354.778745

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **product**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.358230	-0.057870	-0.162543
2	1	0	1.073947	0.394642	0.538743
3	1	0	0.945159	-0.590087	-0.920766
4	6	0	-0.488300	1.003720	-0.798193
5	1	0	-1.053774	1.639277	-0.113011
6	6	0	-0.607800	1.210742	-2.110242
7	1	0	-0.065294	0.605176	-2.834443
8	1	0	-1.244454	1.995559	-2.511451
9	8	0	0.403060	-1.989835	1.248518
10	6	0	-0.468479	-1.078740	0.624707
11	1	0	-1.162691	-1.582726	-0.069722
12	1	0	-1.092202	-0.544011	1.363886
13	50	0	-0.210019	-3.526699	2.295190
14	6	0	1.619863	-4.513581	2.801688
15	1	0	1.440587	-5.334003	3.504177
16	1	0	2.094131	-4.921929	1.904255
17	1	0	2.312016	-3.804325	3.265473
18	6	0	-1.266079	-2.810122	4.025717
19	1	0	-0.638066	-2.125663	4.604163
20	1	0	-2.180084	-2.282520	3.735428
21	1	0	-1.547111	-3.649673	4.670838
22	6	0	-1.500566	-4.738113	1.075033
23	1	0	-0.994470	-5.034873	0.151308
24	1	0	-1.786872	-5.645064	1.618596

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   25          1             0       -2.414051   -4.195231    0.812964

HF=-354.8520877
                     1                      2                      3
                     A                      A                      A
 Frequencies --    21.7381                37.0762                47.8092
 Red. masses --     3.4186                 2.0173                 1.0695
 Frc consts  --     0.0010                 0.0016                 0.0014
 IR Inten    --     0.8325                 0.0363                 0.0028
 Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
   1   6     0.01  -0.03  -0.04    -0.06   0.06   0.07    -0.02   0.02   0.02
   2   1     0.06  -0.11  -0.04    -0.21   0.11   0.20    -0.06   0.04   0.05
   3   1    -0.05   0.00  -0.11     0.12   0.15   0.14     0.03   0.04   0.04
   4   6     0.02   0.06   0.09    -0.07  -0.01  -0.02    -0.03  -0.01  -0.01
   5   1     0.08   0.02   0.17    -0.30  -0.14  -0.09    -0.09  -0.04  -0.03
   6   6    -0.04   0.17   0.11     0.18   0.08  -0.03     0.03   0.00  -0.02
   7   1    -0.10   0.20   0.04     0.41   0.20   0.04     0.10   0.03   0.01
   8   1    -0.02   0.23   0.21     0.16   0.02  -0.10     0.02  -0.02  -0.04
   9   8     0.01  -0.12  -0.17    -0.05  -0.01  -0.02     0.00   0.00   0.00
  10   6     0.01  -0.05  -0.06    -0.06  -0.06  -0.09    -0.01  -0.01  -0.02
  11   1    -0.04   0.02  -0.06     0.08  -0.10  -0.20     0.02  -0.03  -0.04
  12   1     0.06  -0.08   0.00    -0.21  -0.16  -0.14    -0.04  -0.04  -0.03
  13  50     0.00  -0.01  -0.01     0.00  -0.01   0.00     0.00   0.00   0.00
  14   6     0.00   0.05   0.12     0.03   0.02  -0.06    -0.01  -0.02  -0.01
  15   1    -0.03   0.03   0.08     0.10   0.16   0.12    -0.09  -0.38  -0.45
  16   1     0.08   0.09   0.15    -0.10  -0.16  -0.04     0.25   0.46  -0.10
  17   1    -0.06   0.06   0.19     0.11   0.09  -0.28    -0.19  -0.18   0.49
  18   6    -0.02   0.18  -0.10     0.06   0.01   0.04     0.02   0.01   0.01
  19   1    -0.05   0.29  -0.20     0.08   0.03   0.00     0.02   0.02  -0.01
  20   1    -0.05   0.09  -0.16     0.04  -0.01   0.07     0.01  -0.01   0.02
  21   1     0.03   0.26   0.02     0.10   0.01   0.06     0.04   0.01   0.03
  22   6     0.02  -0.16   0.11    -0.04  -0.03   0.07    -0.01   0.01   0.01
  23   1     0.06  -0.33   0.19    -0.06  -0.07   0.07    -0.01  -0.02   0.02
  24   1    -0.05  -0.06   0.25    -0.04  -0.01   0.11    -0.03   0.02   0.03
  25   1     0.06  -0.16  -0.03    -0.03  -0.03   0.06     0.00   0.02   0.00

thermodynamics:
Sum of electronic and zero-point Energies=           -354.639469

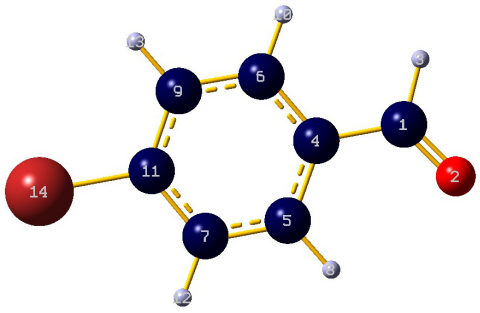
Sum of electronic and thermal Enthalpies=            -354.623004

Sum of electronic and thermal Free Energies=         -354.685549


 Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -354.835389
```

With bromobenzaldehyde

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **bromobenzaldehyde**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.048739	-.000043	-.021837
2	8	0	-.002325	.015356	1.191061
3	1	0	.884481	-.015862	-.628266
4	6	0	-1.297689	.000048	-.812251
5	6	0	-2.540940	.019149	-.166581
6	6	0	-1.242960	-.019110	-2.209517
7	6	0	-3.715362	.019208	-.905980
8	1	0	-2.563826	.033765	.919472
9	6	0	-2.412096	-.019281	-2.963664
10	1	0	-.277610	-.034091	-2.712142
11	6	0	-3.638363	-.000090	-2.300966
12	1	0	-4.683463	.033969	-.416280
13	1	0	-2.378848	-.034012	-4.047854
14	35	0	-5.236216	-.000182	-3.314873

HF=-2916.2205985

	1			2			3		
	A			A			A		
Frequencies --	80.4867			162.8664			169.3563		
Red. masses --	9.7384			9.6940			3.4750		
Frc consts --	.0372			.1515			.0587		
IR Inten --	2.4356			5.4441			6.6960		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	.12	.00	.07	.00	-.10	.00	.27	.00
2 8	.00	.46	-.01	.49	-.01	-.12	.00	-.19	.00
3 1	.00	.08	.00	-.13	.01	-.41	.01	.82	-.01
4 6	.00	-.19	.00	-.12	.00	.18	.00	.12	.00
5 6	.00	-.35	.00	-.13	.00	.19	.00	.04	.00
6 6	.00	-.17	.00	-.15	.00	.19	.00	-.02	.00
7 6	.00	-.37	.01	-.15	.00	.17	.00	-.07	.00
8 1	.00	-.39	.01	-.16	.01	.19	.00	.11	.00
9 6	.00	-.16	.00	-.13	.00	.19	.00	-.21	.00
10 1	.00	-.08	.00	-.15	.00	.19	.00	.00	.00
11 6	.00	-.20	.00	-.14	.00	.16	.00	-.15	.00
12 1	.00	-.45	.01	-.14	.00	.17	.00	-.04	.00
13 1	.00	-.06	.00	-.12	.00	.19	.00	-.33	.00
14 35	.00	.12	.00	.02	.00	-.13	.00	.03	.00

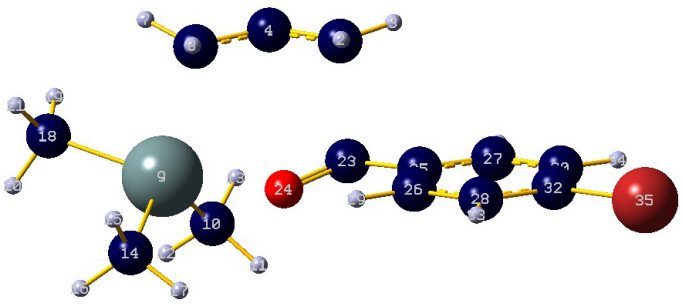
thermodynamics:
Sum of electronic and zero-point Energies= -2916.120151

Sum of electronic and thermal Enthalpies= -2916.111521

Sum of electronic and thermal Free Energies= -2916.153957

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2916.223600

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS$_\gamma$**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.375690	2.047375	-.932332
2	1	0	-.088971	1.470180	-1.727549
3	1	0	-.239434	2.840843	-.516017
4	6	0	1.754859	2.187874	-.936215
5	1	0	2.189043	2.970019	-.309420
6	6	0	2.652313	1.269663	-1.532048
7	1	0	3.658231	1.641213	-1.724294
8	1	0	2.253148	.663651	-2.347398
9	50	0	3.258502	-.343630	.092129
10	6	0	3.173822	.282725	2.154356
11	1	0	2.313670	-.155021	2.668365
12	1	0	4.090574	-.034000	2.663059
13	1	0	3.112208	1.373601	2.235447
14	6	0	3.014816	-2.422205	-.401343
15	1	0	2.948448	-2.548011	-1.487503
16	1	0	3.881315	-2.992276	-.049658
17	1	0	2.104369	-2.821883	.050233
18	6	0	5.370463	.005149	-.391426
19	1	0	5.665626	1.037013	-.166782
20	1	0	6.002233	-.664042	.205635
21	1	0	5.579258	-.189512	-1.449869
22	1	0	.450644	1.172762	1.334281
23	6	0	.179424	.535953	.476288
24	8	0	.959079	-.413428	.144072
25	6	0	-1.293689	.343250	.314466
26	6	0	-1.784805	-.709109	-.465523
27	6	0	-2.198695	1.178271	.977935
28	6	0	-3.153753	-.917027	-.595151
29	1	0	-1.076320	-1.369724	-.956202
30	6	0	-3.571066	.980769	.859713
31	1	0	-1.828591	1.991289	1.599934
32	6	0	-4.037542	-.066616	.067898
33	1	0	-3.535413	-1.735030	-1.197547
34	1	0	-4.272135	1.627252	1.377205
35	35	0	-5.905618	-.345309	-.101162

HF=-3156.5490072

	1			2			3		
	A			A			A		
Frequencies --	-333.5729			29.7894			39.4315		
Red. masses --	10.2619			4.2561			4.6740		
Frc consts --	.6728			.0022			.0043		
IR Inten --	364.3339			.0437			.2772		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.03	.46	-.40	.03	-.03	-.13	-.06	-.10	.04
2 1	-.05	.07	-.05	.09	-.05	-.15	-.09	-.09	.05
3 1	-.02	.30	-.19	-.01	-.04	-.18	-.04	-.11	.08
4 6	-.07	.04	.01	.03	.00	-.06	-.06	-.09	-.04
5 1	-.04	-.03	.09	-.02	.02	-.04	-.02	-.08	-.07
6 6	.00	-.21	.18	.09	.02	.00	-.09	-.09	-.08
7 1	-.09	-.03	-.01	.09	.04	.07	-.10	-.10	-.16
8 1	-.03	.04	.00	.16	.02	-.03	-.14	-.13	-.03
9 50	.05	.02	-.03	.00	.00	.02	.02	.02	-.01
10 6	-.04	-.01	-.01	-.18	-.13	.05	-.06	.07	-.02
11 1	-.02	-.01	.03	-.20	-.21	-.04	-.04	.04	-.02
12 1	-.03	-.01	-.03	-.20	-.12	.10	-.05	.11	.00
13 1	-.04	-.01	-.01	-.24	-.14	.13	-.10	.06	-.04
14 6	-.02	.01	.02	.07	.03	-.11	.19	-.02	.07
15 1	-.02	.01	.02	.05	.09	-.12	.31	-.08	.07
16 1	-.02	.01	.01	.08	.03	-.16	.19	.06	.19
17 1	-.01	-.02	.01	.08	-.03	-.13	.17	-.05	.00
18 6	.07	-.06	.07	.04	.08	.23	.00	.20	.04
19 1	.03	-.04	.03	-.02	.09	.28	-.11	.24	-.01

20	1	.17	-.01	.01	.00	.09	.27	.05	.29	.10
21	1	.03	-.03	.05	.14	.12	.24	.05	.16	.06
22	1	.06	-.01	.00	.01	-.02	-.13	.03	-.16	.02
23	6	-.12	-.37	.34	.01	-.01	-.13	.01	-.13	.01
24	8	-.15	-.09	.08	.00	-.02	-.13	.02	-.12	-.04
25	6	-.04	-.03	.04	.00	.01	-.11	.01	-.13	.04
26	6	-.03	-.02	.00	-.03	.00	-.09	-.03	-.06	-.02
27	6	-.02	.00	.02	.03	.02	-.10	.04	-.15	.11
28	6	-.02	.01	-.02	-.03	.00	-.04	-.04	-.01	-.03
29	1	-.03	-.02	.01	-.05	-.01	-.10	-.05	-.05	-.07
30	6	-.02	.01	.00	.02	.02	-.05	.03	-.09	.10
31	1	-.01	-.01	.03	.05	.03	-.12	.07	-.20	.16
32	6	-.01	.01	-.01	-.01	.01	-.01	-.01	-.02	.02
33	1	-.03	.02	-.03	-.06	-.01	-.01	-.07	.05	-.09
34	1	-.02	.02	-.02	.04	.03	-.03	.05	-.10	.15
35	35	.00	.00	.00	-.01	.00	.08	-.02	.09	-.02

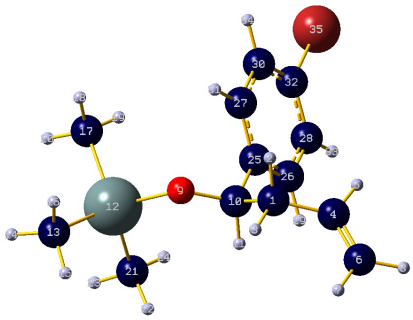
thermodynamics:
Sum of electronic and zero-point Energies= -3156.267242

Sum of electronic and thermal Enthalpies= -3156.245813

Sum of electronic and thermal Free Energies= -3156.318717

Total free energy in solution:
with all non electrostatic terms (a.u.) = -3156.534506

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **product**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.101443	-.040167	.134324
2	1	0	-.284148	.079897	1.211822
3	1	0	.974647	-.206199	.006170
4	6	0	-.533302	1.188172	-.608472
5	1	0	-1.566034	1.505690	-.459875
6	6	0	.248769	1.895706	-1.425404
7	1	0	1.287301	1.620401	-1.602773
8	1	0	-.114292	2.781510	-1.940903
9	8	0	-.235543	-2.386804	.433185
10	6	0	-.813943	-1.338911	-.306680
11	1	0	-.626366	-1.461571	-1.387606
12	50	0	-.395410	-4.294910	-.036342
13	6	0	1.517979	-5.078072	.524826
14	1	0	1.515482	-6.172837	.502914
15	1	0	2.294674	-4.718188	-.156693
16	1	0	1.771392	-4.752937	1.538625
17	6	0	-1.980179	-5.172466	1.114100
18	1	0	-1.803671	-5.032410	2.185014
19	1	0	-2.939468	-4.715099	.855853
20	1	0	-2.040464	-6.247690	.912909
21	6	0	-.782240	-4.446733	-2.143539
22	1	0	-.000998	-3.949679	-2.726836

23	1	0	-.812001	-5.501222	-2.438370
24	1	0	-1.747677	-3.995060	-2.390848
25	6	0	-2.318920	-1.258154	-.107155
26	6	0	-3.174572	-.941104	-1.166377
27	6	0	-2.876980	-1.480574	1.156837
28	6	0	-4.552788	-.842265	-.978285
29	1	0	-2.760828	-.765295	-2.157433
30	6	0	-4.250896	-1.389078	1.363418
31	1	0	-2.221312	-1.740076	1.983538
32	6	0	-5.079212	-1.068803	.289633
33	1	0	-5.209906	-.598153	-1.806597
34	1	0	-4.677148	-1.564615	2.345881
35	35	0	-6.954996	-.946824	.559476

HF=-3156.6030498

		1			2			3		
		A			A			A		
Frequencies --		11.1827			22.0458			39.4033		
Red. masses --		3.1380			6.9366			4.2524		
Frc consts --		.0002			.0020			.0039		
IR Inten --		.0065			.7361			.2242		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.01	.00	-.03	-.08	-.05	.01	.03	.00	.01
2	1	.00	.01	-.03	-.08	-.03	.01	-.03	.10	-.01
3	1	-.01	.00	-.04	-.08	-.05	.01	.03	-.08	.09
4	6	-.01	-.01	-.04	-.08	-.06	-.01	.16	-.03	-.12
5	1	-.01	-.01	-.03	-.07	-.05	.00	.19	.07	-.19
6	6	-.02	-.02	-.06	-.09	-.10	-.05	.26	-.19	-.17
7	1	-.02	-.03	-.07	-.10	-.11	-.06	.24	-.30	-.10
8	1	-.02	-.03	-.07	-.09	-.10	-.06	.35	-.21	-.28
9	8	-.01	.00	.00	-.09	-.04	.06	-.05	.01	.09
10	6	-.01	-.01	-.01	-.08	-.06	.03	-.01	.01	.06
11	1	-.02	-.02	-.01	-.07	-.08	.04	-.02	-.02	.06
12	50	.01	.00	-.01	.09	-.04	.00	-.01	.03	.00
13	6	-.07	-.02	.20	.16	.10	-.04	.00	.03	-.04
14	1	-.08	-.02	.21	.25	.10	-.04	.02	.03	-.08
15	1	.01	-.03	.28	.13	.16	-.05	-.01	.07	-.03
16	1	-.17	-.02	.23	.16	.12	-.04	.00	-.01	-.03
17	6	-.14	.02	-.20	.17	-.20	-.02	.00	-.06	-.04
18	1	-.28	.03	-.18	.24	-.36	-.02	.04	-.18	-.03
19	1	-.11	.01	-.32	.16	-.15	.10	.01	.00	.04
20	1	-.11	.01	-.20	.14	-.17	-.18	-.03	-.03	-.16
21	6	.25	.00	-.05	.10	.00	-.01	-.01	.14	-.01
22	1	.30	.04	.04	.05	.10	.01	-.05	.23	.02
23	1	.33	.00	-.06	.20	.01	-.05	.06	.16	-.08
24	1	.26	-.05	-.17	.06	-.08	.01	-.04	.10	.03
25	6	-.01	.00	.00	-.08	-.05	.02	-.01	.05	.05
26	6	-.02	-.02	.00	-.06	.03	.03	.00	.10	.06
27	6	.00	.02	.01	-.10	-.09	.00	-.03	-.01	.03
28	6	-.02	-.02	.01	-.06	.08	.02	.00	.09	.04
29	1	-.03	-.03	.00	-.04	.06	.04	.01	.15	.07
30	6	.00	.02	.02	-.10	-.04	.00	-.03	-.03	.02
31	1	.01	.03	.01	-.12	-.15	.00	-.04	-.05	.03
32	6	-.01	.00	.02	-.08	.05	.01	-.02	.01	.02
33	1	-.02	-.03	.02	-.04	.15	.03	.00	.12	.05
34	1	.01	.04	.03	-.12	-.07	-.02	-.04	-.08	.01
35	35	.00	.01	.04	-.07	.14	.00	-.03	-.06	.00

thermodynamics:
Sum of electronic and zero-point Energies= -3156.319171

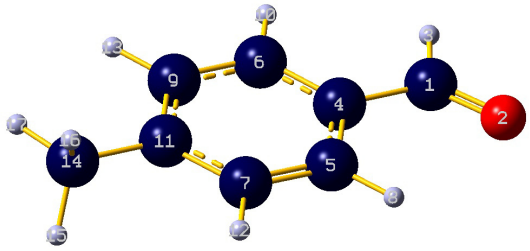
Sum of electronic and thermal Enthalpies= -3156.296876

Sum of electronic and thermal Free Energies= -3156.374855

Total free energy in solution:
with all non electrostatic terms (a.u.) = -3156.584803

With paratolualdehyde

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **paratolualdehyde**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.044975	.000521	-.019148
2	8	0	.009436	-.038386	1.193999
3	1	0	.886811	.040652	-.628147
4	6	0	-1.291970	-.000194	-.807524
5	6	0	-2.538937	-.047724	-.167719
6	6	0	-1.238879	.046716	-2.203129
7	6	0	-3.704334	-.048076	-.917759
8	1	0	-2.564038	-.083917	.917890
9	6	0	-2.412947	.046025	-2.951037
10	1	0	-.272713	.083743	-2.703832
11	6	0	-3.661831	-.000990	-2.321948
12	1	0	-4.669139	-.085443	-.415848
13	1	0	-2.362656	.082256	-4.036932
14	6	0	-4.936898	.000044	-3.121587
15	1	0	-5.541334	-.889128	-2.904265
16	1	0	-5.554129	.874332	-2.880186
17	1	0	-4.738135	.016722	-4.197416

HF=-384.737556

	1			2			3		
	A			A			A		
Frequencies --	29.4567			99.3857			187.2847		
Red. masses --	1.0508			5.1094			2.7152		
Frc consts --	.0005			.0297			.0561		
IR Inten --	.4246			1.4777			8.8584		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	-.02	.00	.00	.00	.00	-.01	.25	.01
2 8	.00	.00	.00	-.01	.33	.01	.00	-.14	.00
3 1	.00	-.04	.00	.00	-.13	.00	-.01	.76	.03
4 6	.00	-.01	.00	.00	-.19	-.01	.00	.07	.00
5 6	.00	.03	.00	.01	-.25	-.01	.00	-.01	.00
6 6	.00	-.02	.00	.00	-.13	.00	.00	-.06	.00
7 6	.00	.04	.00	.00	-.17	-.01	.00	-.05	.00
8 1	.00	.05	.00	.01	-.30	-.01	.00	.04	.00
9 6	.00	-.01	.00	.00	-.02	.00	.00	-.18	-.01
10 1	.00	-.04	.00	.00	-.11	.00	.00	-.04	-.01
11 6	.00	.02	.00	.00	.01	.00	.00	-.07	.00
12 1	.00	.07	.00	.00	-.20	-.01	.00	-.01	.00
13 1	.00	-.01	.00	.00	.09	.00	.00	-.25	-.01
14 6	.00	-.02	.00	-.01	.27	.01	.00	.14	.01
15 1	.29	-.33	-.41	-.07	.27	-.19	-.08	.16	-.14
16 1	-.29	-.34	.40	.06	.27	.22	.08	.16	.16
17 1	.00	.52	.01	-.01	.51	.01	-.01	.30	.01

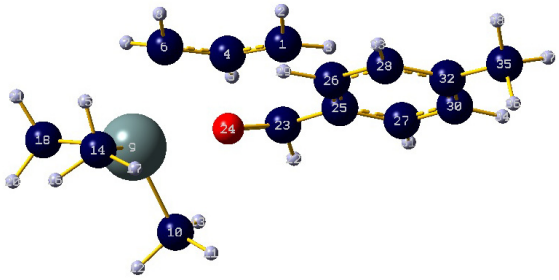
thermodynamics:
Sum of electronic and zero-point Energies= -384.599532

```
Sum of electronic and thermal Enthalpies=            -384.590398

Sum of electronic and thermal Free Energies=         -384.633382

 Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -384.737169
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS$_\gamma$**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.637002	1.997629	-.888980
2	1	0	-1.058266	1.434876	-1.718022
3	1	0	-1.299245	2.740060	-.451433
4	6	0	.733483	2.210150	-.862249
5	1	0	1.115856	2.984165	-.192861
6	6	0	1.687169	1.364014	-1.475601
7	1	0	2.679891	1.787392	-1.623579
8	1	0	1.337291	.775783	-2.325899
9	50	0	2.313697	-.296672	.099534
10	6	0	2.162970	.232276	2.186850
11	1	0	1.307337	-.256774	2.660838
12	1	0	3.078759	-.077748	2.701610
13	1	0	2.062458	1.315451	2.317597
14	6	0	2.197887	-2.366522	-.475896
15	1	0	2.135326	-2.455381	-1.566016
16	1	0	3.098386	-2.895587	-.146235
17	1	0	1.313990	-2.837452	-.040119
18	6	0	4.419644	.168956	-.317832
19	1	0	4.662160	1.205009	-.052920
20	1	0	5.069182	-.491111	.270352
21	1	0	4.658210	.020259	-1.377501
22	1	0	-.551225	1.030118	1.332215
23	6	0	-.786001	.426916	.439774
24	8	0	.042724	-.472307	.075735
25	6	0	-2.246107	.173034	.256390
26	6	0	-2.689453	-.848305	-.590751
27	6	0	-3.192685	.922101	.961802
28	6	0	-4.048620	-1.101467	-.733281
29	1	0	-1.951457	-1.442390	-1.121878
30	6	0	-4.552122	.661231	.817584
31	1	0	-2.862665	1.714349	1.632160
32	6	0	-5.005391	-.354535	-.032170
33	1	0	-4.377499	-1.899714	-1.396165
34	1	0	-5.274369	1.253095	1.376406
35	6	0	-6.474007	-.660596	-.164514
36	1	0	-6.769589	-1.478133	.506738
37	1	0	-7.090678	.208064	.088914
38	1	0	-6.729105	-.971581	-1.183567

```
HF=-625.0644822
                     1                    2                    3
                     A                    A                    A
```

Frequencies --	-345.2692			25.7355			29.5703		
Red. masses --	10.3464			1.8666			1.2655		
Frc consts --	.7267			.0007			.0007		
IR Inten --	370.9550			.1525			.2754		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.02	.48	-.38	.01	-.02	-.04	.00	-.02	-.03
2 1	-.05	.06	-.03	.01	-.03	-.04	.00	-.02	-.03
3 1	-.03	.30	-.17	.00	-.03	-.05	.01	-.01	-.04
4 6	-.07	.04	.01	.01	-.02	-.03	.00	-.02	-.04
5 1	-.04	-.04	.08	.00	-.01	-.03	.01	-.01	-.05
6 6	.01	-.22	.18	.01	-.02	-.02	.00	-.03	-.03
7 1	-.08	-.03	-.01	.01	-.01	-.01	.00	-.03	-.04
8 1	-.03	.05	.00	.02	-.02	-.02	.00	-.04	-.02
9 50	.05	.03	-.03	.00	.00	.00	.00	.00	.00
10 6	-.04	-.01	-.02	-.09	-.06	.01	-.05	-.01	.00
11 1	-.02	-.01	.03	-.12	-.07	-.04	-.06	-.01	-.02
12 1	-.03	-.01	-.04	-.12	-.09	.04	-.06	-.02	.02
13 1	-.03	-.01	-.01	-.08	-.06	.04	-.04	-.01	.01
14 6	-.03	.01	.01	.09	.02	-.06	.05	.00	-.01
15 1	-.03	.01	.01	.31	.04	-.08	.20	.00	-.02
16 1	-.02	.02	.01	.03	.01	.10	.01	.00	.11
17 1	-.01	-.02	.01	.01	.01	-.25	-.01	.01	-.12
18 6	.07	-.06	.07	.00	.08	.12	.00	.04	.06
19 1	.03	-.04	.03	-.05	.09	.12	-.03	.05	.05
20 1	.18	.00	.01	.00	.11	.16	.00	.07	.09
21 1	.02	-.03	.05	.07	.08	.13	.04	.03	.07
22 1	.06	-.01	.00	.03	-.04	-.05	.02	-.01	-.03
23 6	-.11	-.39	.32	.01	-.03	-.05	.01	-.01	-.03
24 8	-.15	-.09	.07	.00	-.03	-.07	.00	-.02	-.03
25 6	-.04	-.03	.03	.00	-.01	-.03	.00	.00	-.01
26 6	-.03	-.02	.00	-.03	-.01	-.01	-.02	.01	-.02
27 6	-.02	.00	.02	.03	.00	-.01	.02	-.01	.01
28 6	-.02	.00	-.02	-.03	.01	.02	-.02	.02	.00
29 1	-.02	-.02	.01	-.05	-.02	-.03	-.03	.01	-.03
30 6	-.02	.01	.00	.02	.02	.02	.01	.00	.03
31 1	-.01	-.01	.02	.05	.00	-.02	.03	-.02	.02
32 6	-.01	.01	.00	-.01	.02	.03	.00	.01	.03
33 1	-.03	.01	-.02	-.06	.01	.03	-.03	.02	.00
34 1	-.02	.02	-.02	.04	.03	.03	.02	-.01	.05
35 6	-.01	.01	.00	-.02	.04	.08	-.01	.02	.03
36 1	.01	.00	.00	-.09	.33	.41	.10	-.34	-.36
37 1	-.01	.00	.01	.01	.17	-.29	-.01	-.13	.53
38 1	.00	.00	.00	.02	-.36	.20	-.10	.53	-.11

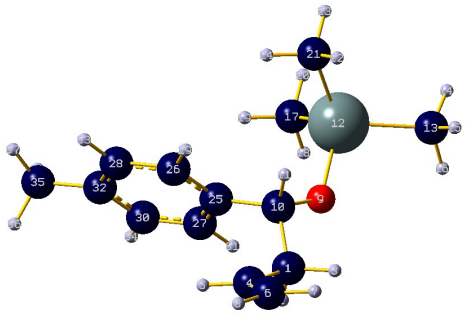
thermodynamics:
Sum of electronic and zero-point Energies= -624.745205

Sum of electronic and thermal Enthalpies= -624.723282

Sum of electronic and thermal Free Energies= -624.797170

Total free energy in solution:
with all non electrostatic terms (a.u.) = -625.046206

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **product**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.068680	-.026728	.139110
2	1	0	-.239535	.080357	1.220098
3	1	0	1.009111	-.167831	-.004615
4	6	0	-.537233	1.198716	-.585527
5	1	0	-1.583451	1.472287	-.443772
6	6	0	.226390	1.951363	-1.379283
7	1	0	1.276332	1.718474	-1.550357
8	1	0	-.164252	2.832768	-1.882214
9	8	0	-.139977	-2.377931	.407898
10	6	0	-.763179	-1.333325	-.304582
11	1	0	-.594331	-1.439388	-1.390437
12	50	0	-.372547	-4.286100	-.019344
13	6	0	1.564741	-5.103336	.397129
14	1	0	1.549471	-6.196789	.338699
15	1	0	2.302064	-4.726955	-.318398
16	1	0	1.883727	-4.815465	1.403703
17	6	0	-1.867346	-5.129266	1.270026
18	1	0	-1.588746	-4.998124	2.320266
19	1	0	-2.832175	-4.642938	1.101607
20	1	0	-1.974644	-6.201658	1.073041
21	6	0	-.929910	-4.467545	-2.086052
22	1	0	-.175964	-4.017905	-2.739586
23	1	0	-1.029419	-5.525190	-2.353034
24	1	0	-1.890425	-3.975310	-2.265664
25	6	0	-2.264497	-1.289460	-.073935
26	6	0	-3.153446	-1.037114	-1.121375
27	6	0	-2.793370	-1.483717	1.208350
28	6	0	-4.529019	-.975621	-.896115
29	1	0	-2.766145	-.886059	-2.127629
30	6	0	-4.165350	-1.424865	1.430233
31	1	0	-2.114703	-1.696008	2.030652
32	6	0	-5.059984	-1.166441	.382234
33	1	0	-5.200506	-.781581	-1.730500
34	1	0	-4.552676	-1.582608	2.435533
35	6	0	-6.543142	-1.084025	.634924
36	1	0	-6.807318	-.153199	1.153958
37	1	0	-7.111127	-1.110629	-.300699
38	1	0	-6.891025	-1.912130	1.263503

HF=-625.1178912

	1			2			3		
	A			A			A		
Frequencies --	14.1469			16.2296			29.4552		
Red. masses --	1.0265			3.2786			4.2675		
Frc consts --	.0001			.0005			.0022		
IR Inten --	.2203			.1452			.7519		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	.00	.00	-.02	-.01	-.03	-.05	-.03	.01
2 1	.00	.00	.00	.00	.00	-.03	-.06	-.02	.01
3 1	.00	.00	.00	-.02	-.02	-.05	-.05	-.05	.03

4	6	.00	.00	.01	-.02	-.02	-.05	-.03	-.04	-.01
5	1	.00	.00	.01	-.01	-.01	-.03	-.02	-.01	-.01
6	6	.00	.01	.01	-.02	-.04	-.07	-.02	-.08	-.04
7	1	.00	.01	.01	-.03	-.06	-.09	-.03	-.12	-.05
8	1	-.01	.01	.01	-.02	-.05	-.08	.00	-.09	-.06
9	8	.00	.00	.00	-.03	-.01	.01	-.08	-.03	.06
10	6	.00	.00	.00	-.03	-.01	.00	-.06	-.04	.03
11	1	.00	.00	.00	-.05	-.03	.00	-.05	-.06	.03
12	50	.00	.00	.00	.02	-.01	-.01	.05	-.03	.01
13	6	.00	.00	.01	-.02	.02	.21	.12	.09	-.09
14	1	-.01	.00	.01	-.02	.01	.33	.19	.09	-.09
15	1	.00	.00	.01	.04	-.07	.22	.06	.14	-.13
16	1	-.01	.00	.01	-.09	.14	.20	.15	.11	-.11
17	6	-.01	.00	-.01	-.11	-.03	-.18	.14	-.14	.04
18	1	-.01	.00	-.01	-.21	-.08	-.15	.20	-.20	.03
19	1	-.01	.00	-.02	-.09	-.02	-.25	.13	-.15	.12
20	1	-.01	.00	-.01	-.11	-.03	-.24	.15	-.14	-.01
21	6	.01	.00	-.01	.23	.00	-.07	-.01	-.01	.02
22	1	.01	.01	.00	.28	.03	.01	-.04	.02	.00
23	1	.01	.00	-.01	.29	.00	-.10	.00	-.01	.01
24	1	.01	.00	-.01	.23	-.03	-.16	-.03	-.03	.06
25	6	.00	.00	.00	-.03	.00	.02	-.07	.00	.01
26	6	.00	-.01	.00	-.04	.00	.03	-.04	.12	.02
27	6	.00	.00	.00	-.01	.02	.03	-.09	-.07	-.01
28	6	.00	-.02	.00	-.04	.03	.05	-.04	.18	.00
29	1	.00	-.02	.00	-.06	-.01	.02	-.02	.17	.03
30	6	.00	.00	.00	-.01	.04	.05	-.10	-.01	-.03
31	1	.00	.01	.00	.00	.02	.02	-.12	-.16	-.02
32	6	.00	-.01	.00	-.02	.05	.06	-.07	.12	-.02
33	1	.00	-.03	.00	-.05	.03	.06	-.01	.28	.01
34	1	.00	.00	.00	.01	.06	.06	-.12	-.06	-.05
35	6	.00	.02	.00	-.01	.07	.09	-.06	.21	-.03
36	1	-.05	.30	-.51	.01	.04	.14	-.02	.26	-.10
37	1	-.03	-.53	.03	-.03	.13	.09	-.06	.18	-.03
38	1	.08	.35	.48	-.03	.04	.05	-.11	.27	.02

thermodynamics:
Sum of electronic and zero-point Energies= -624.796362

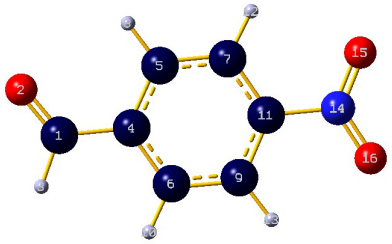
Sum of electronic and thermal Enthalpies= -624.773651

Sum of electronic and thermal Free Energies= -624.852171

Total free energy in solution:
with all non electrostatic terms (a.u.) = -625.095919

With paranitrobenzaldehyde

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **paranitrobenzaldehyde**.



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

1	6	0	-.050750	.000047	-.025091
2	8	0	-.012350	.015938	1.186336
3	1	0	.883040	-.015877	-.628510
4	6	0	-1.305332	-.000035	-.817907
5	6	0	-2.545034	.019101	-.164885
6	6	0	-1.245439	-.019333	-2.215490
7	6	0	-3.719976	.019155	-.902493
8	1	0	-2.562440	.033714	.920748
9	6	0	-2.414519	-.019601	-2.968192
10	1	0	-.279300	-.034245	-2.715252
11	6	0	-3.631279	-.000275	-2.293846
12	1	0	-4.695450	.033825	-.430447
13	1	0	-2.403142	-.034232	-4.051653
14	7	0	-4.873985	-.000208	-3.082055
15	8	0	-5.931279	.017325	-2.466510
16	8	0	-4.767978	-.017623	-4.301172

HF=-549.851239

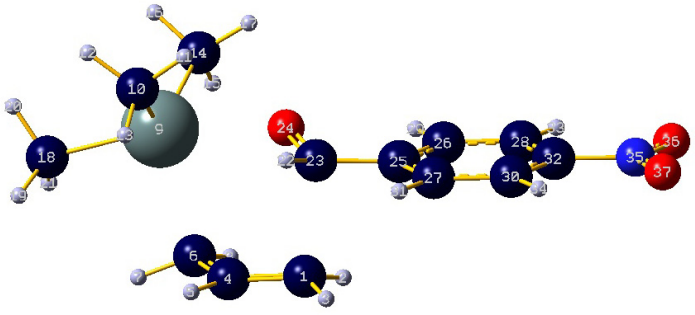
	1			2			3		
	A			A			A		
Frequencies --	56.2473			82.9835			162.6993		
Red. masses --	8.9842			9.0632			3.4705		
Frc consts --	.0167			.0368			.0541		
IR Inten --	1.1489			6.0145			2.8052		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	-.05	.00	.00	.10	.00	.00	.28	.00
2 8	.00	.18	.00	.00	.42	-.01	.00	-.18	.00
3 1	.00	-.25	.00	.00	.05	.00	.01	.83	-.01
4 6	.00	-.07	.00	.00	-.19	.00	.00	.11	.00
5 6	.00	.12	.00	.00	-.36	.00	.00	.04	.00
6 6	.00	-.25	.00	.00	-.12	.00	.00	-.04	.00
7 6	.00	.11	.00	.00	-.35	.00	.00	-.06	.00
8 1	.00	.26	.00	.00	-.43	.01	.00	.11	.00
9 6	.00	-.20	.00	.00	-.09	.00	.00	-.21	.00
10 1	.00	-.40	.01	.00	-.01	.00	.00	-.01	.00
11 6	.00	-.02	.00	.00	-.16	.00	.00	-.14	.00
12 1	.00	.23	.00	.00	-.43	.01	.00	-.03	.00
13 1	.00	-.29	.00	.00	.03	.00	.00	-.30	.01
14 7	.00	.03	.00	.00	.09	.00	.00	.00	.00
15 8	.00	-.40	.01	.00	.28	.00	.00	.07	.00
16 8	.00	.49	-.01	.00	.14	.00	.00	.09	.00

thermodynamics:
Sum of electronic and zero-point Energies= -549.738064

Sum of electronic and thermal Enthalpies= -549.728309

Sum of electronic and thermal Free Energies= -549.772941
Total free energy in solution:
with all non electrostatic terms (a.u.) = -549.855562

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS$_\gamma$**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.084082	-1.907629	-1.153436
2	1	0	.536795	-1.232305	-1.874769
3	1	0	.713433	-2.730746	-.825558
4	6	0	-1.292156	-2.061806	-1.162198
5	1	0	-1.712322	-2.915380	-.625908
6	6	0	-2.206273	-1.096776	-1.651877
7	1	0	-3.202544	-1.467234	-1.891964
8	1	0	-1.818036	-.396561	-2.393745
9	50	0	-2.873014	.307468	.129096
10	6	0	-2.789615	-.554518	2.103143
11	1	0	-1.905629	-.221647	2.653699
12	1	0	-3.684731	-.253313	2.658001
13	1	0	-2.785362	-1.649135	2.057656
14	6	0	-2.651954	2.430311	-.116637
15	1	0	-2.623007	2.686847	-1.181127
16	1	0	-3.509966	2.944618	.329225
17	1	0	-1.730189	2.779983	.352637
18	6	0	-4.970752	-.015613	-.419035
19	1	0	-5.252445	-1.071234	-.327191
20	1	0	-5.620232	.565779	.246813
21	1	0	-5.170863	.304902	-1.448052
22	1	0	-.012973	-1.285659	1.212425
23	6	0	.244545	-.543739	.439045
24	8	0	-.549395	.418859	.214722
25	6	0	1.713811	-.317613	.280943
26	6	0	2.177698	.814178	-.402244
27	6	0	2.634147	-1.199866	.861709
28	6	0	3.539478	1.053594	-.522936
29	1	0	1.451491	1.503770	-.820732
30	6	0	3.999522	-.970935	.753333
31	1	0	2.276628	-2.070275	1.407687
32	6	0	4.432743	.154267	.056187
33	1	0	3.922802	1.921880	-1.046488
34	1	0	4.729865	-1.637899	1.196414
35	7	0	5.871101	.402850	-.064654
36	8	0	6.224617	1.398883	-.684571
37	8	0	6.632106	-.401853	.460197

HF=-790.1825347

	1			2			3		
	A			A			A		
Frequencies --	-308.4673			35.2484			37.2110		
Red. masses --	10.0738			3.9230			4.7722		
Frc consts --	.5648			.0029			.0039		
IR Inten --	286.5928			.4774			.4706		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.02	.41	.45	-.03	.06	-.13	.04	.06	.04
2 1	-.06	.08	.07	-.07	.08	-.13	.09	.05	.06
3 1	-.03	.29	.25	.01	.06	-.16	.01	.05	.07
4 6	-.07	.04	.00	-.02	.03	-.07	.03	.09	-.04
5 1	-.04	-.02	-.08	.02	.01	-.06	-.01	.08	-.08
6 6	.00	-.18	-.21	-.07	.01	-.02	.08	.11	-.08
7 1	-.09	-.04	.00	-.07	-.01	.03	.09	.14	-.16
8 1	-.03	.02	-.02	-.12	.02	-.03	.15	.14	-.01
9 50	.05	.02	.04	.00	.00	.02	.00	-.01	.00
10 6	-.04	-.01	.01	.15	.07	.04	.01	-.13	-.05
11 1	-.02	-.01	-.03	.19	.09	-.03	-.02	-.12	-.01
12 1	-.03	-.02	.02	.19	.09	.09	-.02	-.20	-.05
13 1	-.03	-.01	.00	.15	.07	.08	.06	-.13	-.11
14 6	-.02	.01	-.01	-.10	-.01	-.09	-.11	.02	.17
15 1	-.03	.01	-.01	-.34	-.03	-.10	-.16	.12	.19
16 1	-.02	.01	-.01	-.02	-.02	.09	-.12	-.07	.25
17 1	-.01	-.02	-.02	-.01	.03	-.29	-.12	.02	.17
18 6	.07	-.05	-.07	-.03	-.12	.20	.02	-.09	-.05

19	1	.04	-.04	-.04	.03	-.14	.26	.08	-.12	-.14
20	1	.16	-.01	-.02	.00	-.14	.25	-.02	-.19	-.01
21	1	.04	-.03	-.05	-.15	-.16	.21	.01	-.02	-.02
22	1	.06	-.02	-.01	-.02	.04	-.12	-.02	.09	.03
23	6	-.11	-.31	-.37	-.01	.04	-.11	-.01	.08	.03
24	8	-.15	-.09	-.10	.01	.05	-.12	-.01	.08	.00
25	6	-.04	-.03	-.04	.00	.02	-.09	-.01	.07	.05
26	6	-.03	-.01	.00	.04	.00	-.10	.02	.00	-.06
27	6	-.02	.00	-.02	-.03	.01	-.05	-.03	.11	.14
28	6	-.02	.00	.02	.05	-.02	-.04	.02	-.04	-.08
29	1	-.03	-.02	-.01	.06	.00	-.14	.03	-.02	-.12
30	6	-.02	.01	.01	-.03	.00	.01	-.02	.07	.12
31	1	-.01	-.01	-.03	-.07	.03	-.05	-.05	.17	.22
32	6	-.01	.01	.01	.01	-.01	.01	.00	-.01	.00
33	1	-.03	.01	.03	.08	-.03	-.04	.04	-.11	-.17
34	1	-.03	.01	.02	-.05	.00	.05	-.04	.10	.19
35	7	-.01	.00	.00	.02	-.02	.09	.01	-.07	-.04
36	8	.00	.00	.00	.06	-.04	.08	.03	-.19	-.22
37	8	-.01	.00	.00	-.01	-.01	.16	-.01	.00	.10

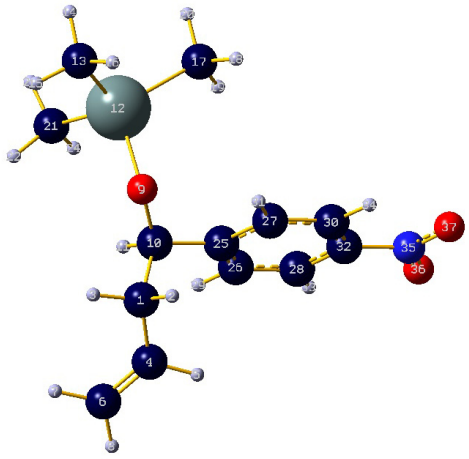
thermodynamics:
Sum of electronic and zero-point Energies= -789.887919

Sum of electronic and thermal Enthalpies= -789.865388

Sum of electronic and thermal Free Energies= -789.940372

Total free energy in solution:
with all non electrostatic terms (a.u.) = -790.170116

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **product**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.125750	-.091181	-.053821
2	1	0	-.166542	.069468	1.032799
3	1	0	.922711	-.279182	-.312863
4	6	0	-.636101	1.115301	-.783081
5	1	0	-1.625681	1.473615	-.497168
6	6	0	.029806	1.759210	-1.743052
7	1	0	1.022758	1.444385	-2.060338
8	1	0	-.386273	2.631018	-2.241837
9	8	0	-.258742	-2.426217	.361791
10	6	0	-.899242	-1.397867	-.349961
11	1	0	-.847134	-1.564675	-1.440150
12	50	0	-.312146	-4.329386	-.159023
13	6	0	1.325271	-5.135314	.956781

14	1	0	1.349624	-6.227332	.882619
15	1	0	2.273989	-4.739186	.582822
16	1	0	1.228946	-4.862153	2.012012
17	6	0	-2.196555	-5.189673	.402558
18	1	0	-2.405324	-5.009364	1.461113
19	1	0	-3.010068	-4.760379	-.189584
20	1	0	-2.178745	-6.271816	.232683
21	6	0	-.027742	-4.419888	-2.286604
22	1	0	.846173	-3.834369	-2.588173
23	1	0	.131110	-5.458393	-2.596388
24	1	0	-.905749	-4.038684	-2.817204
25	6	0	-2.366110	-1.277968	.031044
26	6	0	-3.337211	-.955229	-.924620
27	6	0	-2.761455	-1.468659	1.361809
28	6	0	-4.675170	-.817801	-.569154
29	1	0	-3.041606	-.807886	-1.960869
30	6	0	-4.092432	-1.335847	1.736296
31	1	0	-2.009740	-1.733656	2.099248
32	6	0	-5.033253	-1.010988	.761414
33	1	0	-5.438953	-.571504	-1.297782
34	1	0	-4.415698	-1.479013	2.761054
35	7	0	-6.439609	-.874524	1.146255
36	8	0	-7.244603	-.587505	.267619
37	8	0	-6.726538	-1.055345	2.324000

HF=-790.2374466

		1			2			3		
		A			A			A		
Frequencies --		15.6165			21.8015			33.8262		
Red. masses --		3.3350			5.6931			6.1907		
Frc consts --		.0005			.0016			.0042		
IR Inten --		.1288			.8884			.1481		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-.02	-.01	-.04	-.06	-.05	.01	.03	.03	-.05
2	1	-.01	.00	-.04	-.06	-.04	.01	.03	.04	-.06
3	1	-.03	-.02	-.05	-.06	-.06	.01	.03	.03	-.06
4	6	-.03	-.02	-.05	-.05	-.05	-.01	.03	.03	-.06
5	1	-.02	-.01	-.04	-.04	-.02	.01	.05	.06	-.04
6	6	-.04	-.04	-.07	-.06	-.09	-.04	.02	-.01	-.11
7	1	-.05	-.05	-.08	-.07	-.12	-.05	.00	-.04	-.13
8	1	-.05	-.05	-.08	-.05	-.09	-.05	.02	-.01	-.11
9	8	-.02	-.01	.00	-.08	-.04	.04	.04	.04	-.05
10	6	-.03	-.02	-.01	-.07	-.05	.02	.03	.03	-.04
11	1	-.04	-.03	-.01	-.07	-.06	.03	.02	.03	-.04
12	50	.02	.00	-.01	.07	-.03	.00	-.03	.02	.02
13	6	-.11	-.02	.17	.16	.08	-.07	-.07	.01	.07
14	1	-.11	-.02	.18	.22	.08	-.05	-.11	.01	.13
15	1	-.07	-.02	.28	.12	.12	-.13	-.05	-.04	.06
16	1	-.23	-.01	.16	.20	.09	-.07	-.07	.07	.06
17	6	-.05	.00	-.24	.15	-.18	.05	-.06	.10	.05
18	1	-.17	-.03	-.25	.20	-.27	.07	-.09	.19	.02
19	1	.02	.04	-.31	.09	-.19	.12	-.04	.06	-.01
20	1	-.05	.01	-.28	.20	-.17	-.03	-.07	.08	.14
21	6	.25	.01	.02	.01	.04	-.01	-.02	-.08	.03
22	1	.28	.02	.12	-.04	.11	-.03	.02	-.15	.01
23	1	.30	.01	.03	.08	.05	-.04	-.10	-.10	.07
24	1	.31	.00	-.07	-.04	-.02	.02	.00	-.04	.01
25	6	-.02	-.01	.01	-.07	-.03	.01	.03	.03	-.03
26	6	-.03	.00	.02	-.04	.10	.03	.04	.18	.01
27	6	-.01	-.01	.01	-.10	-.11	-.01	.02	-.15	-.05
28	6	-.03	.02	.03	-.04	.15	.02	.04	.16	.03
29	1	-.04	.00	.01	-.02	.16	.04	.05	.32	.04
30	6	-.01	.01	.02	-.10	-.06	-.01	.02	-.19	-.04
31	1	-.01	-.01	.00	-.12	-.20	-.02	.02	-.25	-.09
32	6	-.01	.02	.04	-.07	.07	.00	.03	-.03	.00

33	1	-.03	.02	.04	-.01	.25	.03	.05	.28	.06
34	1	.00	.01	.03	-.12	-.12	-.03	.01	-.33	-.07
35	7	-.01	.03	.05	-.06	.13	.00	.03	-.08	.01
36	8	-.01	.04	.06	-.03	.27	.01	.05	.17	.06
37	8	.00	.03	.05	-.09	.04	-.02	.00	-.38	-.05

thermodynamics:
Sum of electronic and zero-point Energies= -789.940671

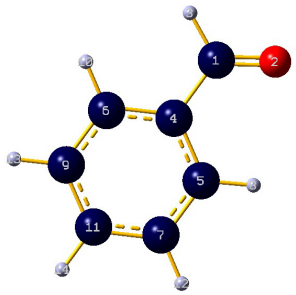
Sum of electronic and thermal Enthalpies= -789.917319

Sum of electronic and thermal Free Energies= -789.997154

Total free energy in solution:
with all non electrostatic terms (a.u.) = -790.220534

With benzaldehyde

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **benzaldehyde**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.049619	-.000138	-.022717
2	8	0	.004034	.015552	1.190235
3	1	0	.882019	-.016243	-.632611
4	6	0	-1.299944	.000065	-.811043
5	6	0	-2.542495	.019178	-.163434
6	6	0	-1.240680	-.019080	-2.208637
7	6	0	-3.712792	.019147	-.911759
8	1	0	-2.560864	.033696	.922716
9	6	0	-2.414201	-.019102	-2.958225
10	1	0	-.271513	-.034009	-2.704432
11	6	0	-3.648694	-.000004	-2.308542
12	1	0	-4.678446	.033984	-.413191
13	1	0	-2.369233	-.033945	-4.043901
14	1	0	-4.566214	.000005	-2.891742

HF=-345.4328128

	1			2			3		
	A			A			A		
Frequencies --	124.3522			216.9526			239.4237		
Red. masses --	5.1678			5.6455			2.4038		
Frc consts --	.0471			.1566			.0812		
IR Inten --	4.0439			7.8076			7.0453		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	-.16	.00	-.01	.00	-.03	.00	.23	.00
2 8	.00	.35	.00	.39	.00	-.05	.00	-.06	.00
3 1	.00	-.52	.01	-.19	.00	-.31	.01	.83	-.01
4 6	.00	-.24	.00	-.16	.00	.17	.00	-.10	.00
5 6	.00	-.24	.00	-.24	.00	.04	.00	-.13	.00
6 6	.00	-.10	.00	-.03	.00	.18	.00	-.13	.00
7 6	.00	-.05	.00	-.14	.00	-.14	.00	.04	.00

8	1	.00	-.34	.00	-.41	.00	.03	.00	-.16	.00
9	6	.00	.15	.00	.09	.00	.02	.00	-.05	.00
10	1	.00	-.12	.00	.04	.00	.31	.00	-.15	.00
11	6	.00	.19	.00	.01	.00	-.13	.00	.14	.00
12	1	.00	-.04	.00	-.21	.00	-.26	.00	.14	.00
13	1	.00	.33	.00	.24	.00	.02	.00	-.06	.00
14	1	.00	.40	-.01	.08	.00	-.24	.00	.33	.00

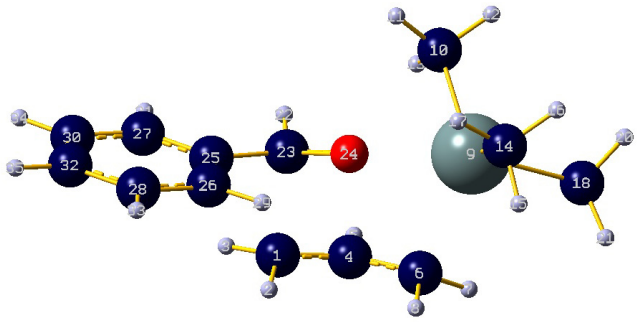
thermodynamics:
Sum of electronic and zero-point Energies= -345.322342

Sum of electronic and thermal Enthalpies= -345.315092

Sum of electronic and thermal Free Energies= -345.352881

Total free energy in solution:
with all non electrostatic terms (a.u.) = -345.435925

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS$_\gamma$**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.054109	1.928212	-0.882619
2	1	0	-1.447471	1.362517	-1.723230
3	1	0	-1.748164	2.635412	-0.436116
4	6	0	0.306586	2.191757	-0.840072
5	1	0	0.653710	2.969889	-0.156412
6	6	0	1.297446	1.391469	-1.457459
7	1	0	2.272514	1.857363	-1.595357
8	1	0	0.976085	0.800029	-2.316687
9	50	0	1.982207	-0.253244	0.105308
10	6	0	1.766378	0.221622	2.199901
11	1	0	0.911618	-0.295301	2.644703
12	1	0	2.677210	-0.081353	2.727615
13	1	0	1.642187	1.299584	2.351633
14	6	0	1.994111	-2.309699	-0.523888
15	1	0	2.105015	-2.371489	-1.611987
16	1	0	2.845947	-2.828911	-0.071370
17	1	0	1.066188	-2.808762	-0.237019
18	6	0	4.069950	0.333087	-0.248420
19	1	0	4.250092	1.375512	0.040406
20	1	0	4.739097	-0.301720	0.345602
21	1	0	4.344509	0.217462	-1.303534
22	1	0	-0.938681	0.914813	1.323119
23	6	0	-1.146845	0.320047	0.418585
24	8	0	-0.283415	-0.537677	0.039870
25	6	0	-2.597330	0.020732	0.219040
26	6	0	-2.996742	-0.992781	-0.659082
27	6	0	-3.566829	0.719519	0.946738
28	6	0	-4.347176	-1.290254	-0.815818
29	1	0	-2.232799	-1.545340	-1.198135
30	6	0	-4.917668	0.418695	0.792258

31	1	0	-3.258835	1.498463	1.642539
32	6	0	-5.311480	-0.585059	-0.093105
33	1	0	-4.650424	-2.080763	-1.497947
34	1	0	-5.663150	0.964145	1.365508
35	1	0	-6.365459	-0.822013	-0.214034

HF=-585.7604405

	1			2			3		
	A			A			A		
Frequencies --	-339.1221			35.5486			47.6224		
Red. masses --	10.2973			2.7470			3.3974		
Frc consts --	0.6977			0.0020			0.0045		
IR Inten --	326.2354			0.0265			0.0175		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.49	-0.37	0.01	-0.04	-0.09	0.01	-0.01	0.02
2 1	-0.05	0.05	-0.04	0.03	-0.06	-0.08	-0.04	0.01	0.03
3 1	-0.04	0.30	-0.17	0.00	-0.04	-0.11	0.04	0.00	0.05
4 6	-0.07	0.04	0.01	0.01	-0.03	-0.08	0.01	-0.04	-0.04
5 1	-0.04	-0.04	0.08	-0.01	-0.01	-0.09	0.06	-0.04	-0.06
6 6	0.02	-0.22	0.18	0.02	-0.04	-0.04	-0.03	-0.07	-0.07
7 1	-0.08	-0.04	-0.01	0.02	-0.03	-0.04	-0.03	-0.10	-0.12
8 1	-0.03	0.04	0.00	0.04	-0.06	-0.04	-0.08	-0.09	-0.03
9 50	0.05	0.03	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
10 6	-0.04	-0.01	-0.02	-0.12	-0.10	0.01	-0.03	0.11	-0.02
11 1	-0.02	-0.01	0.03	-0.14	-0.13	-0.05	-0.03	0.13	0.00
12 1	-0.03	-0.01	-0.04	-0.14	-0.12	0.04	-0.03	0.13	-0.01
13 1	-0.03	-0.01	-0.01	-0.13	-0.11	0.06	-0.02	0.12	-0.08
14 6	-0.03	0.01	0.01	0.11	0.04	-0.10	0.06	-0.04	0.15
15 1	-0.02	0.01	0.01	0.45	0.09	-0.07	0.16	-0.13	0.17
16 1	-0.02	0.01	0.01	-0.05	-0.02	0.13	0.02	0.00	0.27
17 1	-0.01	-0.03	0.01	0.00	0.05	-0.41	0.04	-0.03	0.11
18 6	0.07	-0.06	0.07	0.00	0.11	0.18	-0.01	0.03	-0.01
19 1	0.04	-0.04	0.03	-0.09	0.12	0.21	-0.04	0.05	-0.07
20 1	0.18	0.01	0.02	-0.02	0.14	0.23	-0.01	0.08	0.04
21 1	0.03	-0.03	0.05	0.10	0.14	0.20	0.00	-0.03	0.00
22 1	0.06	-0.01	0.00	0.05	-0.01	-0.07	0.03	-0.06	0.00
23 6	-0.09	-0.40	0.31	0.02	-0.02	-0.06	0.01	-0.04	-0.01
24 8	-0.14	-0.11	0.07	0.00	-0.03	-0.08	0.01	-0.04	-0.04
25 6	-0.04	-0.04	0.03	0.01	0.00	-0.02	0.01	-0.02	0.00
26 6	-0.03	-0.02	0.00	-0.04	-0.01	0.01	-0.03	0.12	-0.15
27 6	-0.02	0.00	0.02	0.04	0.02	0.01	0.04	-0.13	0.14
28 6	-0.02	0.01	-0.02	-0.05	0.01	0.07	-0.03	0.15	-0.15
29 1	-0.03	-0.03	0.01	-0.07	-0.03	-0.01	-0.05	0.20	-0.26
30 6	-0.02	0.02	0.00	0.03	0.04	0.07	0.03	-0.10	0.14
31 1	-0.01	-0.01	0.02	0.08	0.03	-0.01	0.07	-0.24	0.25
32 6	-0.01	0.01	0.00	-0.01	0.03	0.10	0.00	0.05	0.00
33 1	-0.03	0.02	-0.02	-0.09	0.01	0.09	-0.06	0.27	-0.26
34 1	-0.02	0.02	-0.01	0.06	0.06	0.09	0.06	-0.19	0.26
35 1	-0.01	0.02	0.00	-0.02	0.05	0.14	-0.01	0.07	0.00

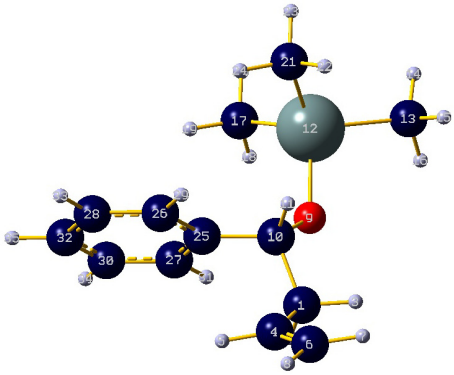
thermodynamics:
Sum of electronic and zero-point Energies= -585.468518

Sum of electronic and thermal Enthalpies= -585.448614

Sum of electronic and thermal Free Energies= -585.516660

Total free energy in solution:
with all non electrostatic terms (a.u.) = -585.745783

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **product**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.098688	-.023311	.161290
2	1	0	-.312773	.083947	1.234468
3	1	0	.982706	-.174049	.061387
4	6	0	-.526267	1.207031	-.580275
5	1	0	-1.573207	1.494097	-.475713
6	6	0	.274478	1.949440	-1.346631
7	1	0	1.326922	1.703559	-1.479955
8	1	0	-.087092	2.835164	-1.863476
9	8	0	-.202866	-2.374090	.426112
10	6	0	-.784725	-1.324364	-.311737
11	1	0	-.571043	-1.431730	-1.389516
12	50	0	-.413425	-4.281078	-.019782
13	6	0	1.509873	-5.093799	.464537
14	1	0	1.492706	-6.188286	.433032
15	1	0	2.266511	-4.737232	-.240928
16	1	0	1.803675	-4.781456	1.471478
17	6	0	-1.953100	-5.130747	1.210853
18	1	0	-1.720821	-4.990002	2.271047
19	1	0	-2.915206	-4.656354	.998254
20	1	0	-2.040988	-6.205473	1.017004
21	6	0	-.895835	-4.452613	-2.105821
22	1	0	-.120823	-3.997189	-2.730003
23	1	0	-.982145	-5.509193	-2.381444
24	1	0	-1.851147	-3.962769	-2.316913
25	6	0	-2.294700	-1.266391	-.143960
26	6	0	-3.131205	-.986763	-1.229368
27	6	0	-2.873663	-1.472561	1.114291
28	6	0	-4.514677	-.910858	-1.064801
29	1	0	-2.693486	-.824586	-2.212810
30	6	0	-4.254791	-1.400105	1.281764
31	1	0	-2.227392	-1.701201	1.957864
32	6	0	-5.080350	-1.118300	.191956
33	1	0	-5.150181	-.694860	-1.920397
34	1	0	-4.689594	-1.563612	2.265148
35	1	0	-6.158321	-1.063693	.322377

HF=-585.8141399

	1			2			3		
	A			A			A		
Frequencies --	15.2016			30.7564			47.3095		
Red. masses --	3.3457			4.4335			3.2881		
Frc consts --	.0005			.0025			.0043		
IR Inten --	.0530			.9902			.0247		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	-.01	-.04	-.04	-.04	.00	.02	.02	-.03
2 1	.03	.01	-.04	-.06	.01	.00	.04	.00	-.02
3 1	-.01	-.02	-.07	-.05	-.08	.03	.02	.04	-.05
4 6	-.01	-.02	-.05	.02	-.05	-.05	-.02	.02	.00
5 1	.00	.00	-.03	.03	.01	-.05	-.01	.03	.07
6 6	-.02	-.04	-.09	.05	-.13	-.09	-.07	.01	-.06

7	1	-.03	-.05	-.11	.04	-.19	-.08	-.08	.00	-.13
8	1	-.03	-.05	-.09	.10	-.13	-.13	-.09	.01	-.04
9	8	-.02	.00	.00	-.12	-.02	.07	.05	.02	-.05
10	6	-.03	-.01	.00	-.08	-.03	.03	.03	.01	-.03
11	1	-.05	-.03	-.01	-.07	-.07	.04	.02	.02	-.03
12	50	.01	.00	-.01	.04	-.02	.01	-.01	.01	.01
13	6	-.04	.00	.20	.11	.10	-.06	-.04	-.03	.07
14	1	-.05	.00	.26	.19	.10	-.06	-.06	-.03	.05
15	1	.02	-.06	.24	.06	.16	-.08	-.01	-.04	.10
16	1	-.12	.06	.20	.12	.13	-.07	-.07	-.05	.08
17	6	-.13	-.01	-.19	.12	-.16	.01	-.04	.07	.02
18	1	-.24	-.03	-.16	.18	-.27	.01	-.15	.28	.01
19	1	-.10	.00	-.29	.10	-.14	.11	-.07	-.08	-.15
20	1	-.11	-.01	-.22	.11	-.14	-.09	.10	.02	.20
21	6	.23	.00	-.07	.01	.01	.01	.00	-.03	.01
22	1	.28	.03	.02	-.01	.05	.01	.04	-.11	.00
23	1	.30	.00	-.09	.04	.02	-.01	-.08	-.04	.05
24	1	.24	-.04	-.16	.00	-.01	.04	.03	.03	-.01
25	6	-.02	.01	.03	-.08	.02	.01	.03	-.01	-.02
26	6	-.05	.00	.05	-.04	.16	.02	.03	.17	.03
27	6	.01	.03	.05	-.11	-.05	-.01	.03	-.21	-.05
28	6	-.04	.02	.08	-.04	.24	.01	.03	.16	.04
29	1	-.07	-.02	.04	-.02	.21	.04	.03	.33	.05
30	6	.01	.05	.08	-.11	.02	-.03	.03	-.23	-.04
31	1	.03	.03	.04	-.13	-.15	-.02	.03	-.34	-.09
32	6	-.01	.04	.10	-.07	.17	-.02	.03	-.05	.01
33	1	-.06	.01	.10	-.01	.35	.02	.03	.30	.08
34	1	.03	.07	.10	-.13	-.03	-.05	.03	-.40	-.07
35	1	-.01	.06	.13	-.07	.22	-.03	.03	-.07	.02

thermodynamics:
Sum of electronic and zero-point Energies= -585.520153

Sum of electronic and thermal Enthalpies= -585.499363

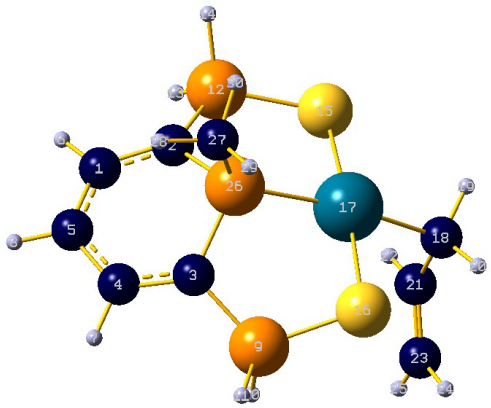
Sum of electronic and thermal Free Energies= -585.572210

Total free energy in solution:
with all non electrostatic terms (a.u.) = -585.796074

II. Mechanism involving a η^1-allyl palladium complex

S~P~*S* complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A1.**



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

1	6	0	3.271789	0.447532	1.088251
2	6	0	2.223705	0.909368	0.292807
3	6	0	1.432536	-1.724348	0.323265
4	6	0	2.557924	-1.901874	1.119294
5	6	0	3.520722	-0.906081	1.363119
6	1	0	3.902263	1.171301	1.608866
7	1	0	2.675780	-2.836314	1.673286
8	1	0	4.379535	-1.157534	1.977569
9	15	0	-0.067927	-2.655846	0.446161
10	1	0	-0.529665	-2.698740	1.785329
11	1	0	0.188001	-4.031160	0.233451
12	15	0	1.541161	2.529764	0.354332
13	1	0	1.869784	3.111565	1.602576
14	1	0	2.220926	3.427384	-0.506031
15	16	0	-0.452517	2.625682	-0.051855
16	16	0	-1.502217	-2.022739	-0.834290
17	46	0	-1.011332	0.333094	-0.541493
18	6	0	-3.016936	0.748371	-0.124372
19	1	0	-3.201976	1.750886	-0.525354
20	1	0	-3.618560	0.007097	-0.658486
21	6	0	-3.164010	0.671092	1.335982
22	1	0	-2.777381	1.522744	1.898606
23	6	0	-3.704520	-0.351967	2.021335
24	1	0	-4.106220	-1.226867	1.513751
25	1	0	-3.768188	-0.339465	3.106661
26	15	0	1.262305	-0.248909	-0.687933
27	6	0	2.248904	-0.578041	-2.210250
28	1	0	3.267586	-0.890185	-1.958551
29	1	0	1.755461	-1.368648	-2.785902
30	1	0	2.285882	0.329052	-2.823774

HF=-2298.8263281

	1			2			3		
	A			A			A		
Frequencies --	18.5060			35.8712			46.7377		
Red. masses --	4.5953			5.0859			4.3188		
Frc consts --	0.0009			0.0039			0.0056		
IR Inten --	0.7542			2.0220			3.7143		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	-0.01	0.02	-0.07	-0.01	0.08	-0.08	0.03	0.10
2 6	-0.03	-0.01	0.05	-0.04	0.00	0.05	-0.01	0.00	-0.01
3 6	0.05	-0.03	-0.05	-0.04	0.00	0.00	0.00	-0.01	0.00
4 6	0.07	-0.03	-0.07	-0.07	-0.01	0.03	-0.06	0.03	0.10
5 6	0.04	-0.01	-0.04	-0.07	-0.01	0.07	-0.10	0.05	0.17
6 1	-0.02	-0.01	0.04	-0.10	-0.01	0.12	-0.12	0.06	0.12
7 1	0.11	-0.05	-0.11	-0.09	-0.01	0.03	-0.09	0.04	0.12
8 1	0.05	-0.01	-0.06	-0.09	-0.01	0.10	-0.16	0.07	0.26
9 15	0.10	-0.11	-0.08	-0.05	0.02	-0.03	0.05	-0.10	-0.13
10 1	0.20	-0.31	-0.05	-0.09	0.05	-0.04	0.08	-0.32	-0.13
11 1	0.13	-0.08	-0.27	-0.05	0.01	0.01	0.08	-0.06	-0.33
12 15	-0.04	-0.01	0.10	-0.05	0.00	0.07	0.03	0.02	-0.16
13 1	-0.18	-0.10	0.18	-0.19	-0.08	0.14	0.22	0.19	-0.29
14 1	0.04	0.06	0.24	0.04	0.05	0.20	-0.07	-0.13	-0.40
15 16	0.00	0.01	-0.11	0.00	0.02	-0.16	-0.03	-0.01	0.11
16 16	-0.01	-0.02	0.08	-0.01	0.00	-0.08	0.01	0.01	-0.04
17 46	-0.01	-0.02	0.01	-0.01	-0.01	-0.03	0.00	0.00	0.01
18 6	-0.02	0.01	-0.05	0.02	-0.03	0.09	0.01	0.00	0.03
19 1	-0.01	-0.03	-0.17	-0.04	-0.05	0.09	0.00	-0.03	-0.02
20 1	-0.01	-0.05	0.02	-0.02	-0.06	0.17	0.01	-0.03	0.08
21 6	-0.05	0.18	-0.05	0.19	0.00	0.11	0.02	0.07	0.04
22 1	-0.07	0.24	-0.14	0.22	0.03	0.04	0.03	0.09	0.00
23 6	-0.07	0.25	0.05	0.31	0.00	0.21	0.02	0.10	0.09
24 1	-0.05	0.19	0.14	0.28	-0.03	0.28	0.02	0.08	0.14
25 1	-0.09	0.37	0.05	0.44	0.02	0.21	0.03	0.15	0.09
26 15	-0.01	0.01	0.02	0.00	0.01	-0.01	0.01	-0.01	-0.01
27 6	-0.02	0.10	-0.01	0.08	0.02	0.04	0.01	-0.01	-0.01
28 1	0.00	0.14	-0.04	0.07	0.02	0.10	0.01	-0.02	0.00

```
  29   1     0.01    0.11  -0.03     0.12    0.01    0.02     0.01  -0.01  -0.01
  30   1    -0.07    0.13   0.03     0.11    0.02    0.05     0.02  -0.01   0.00

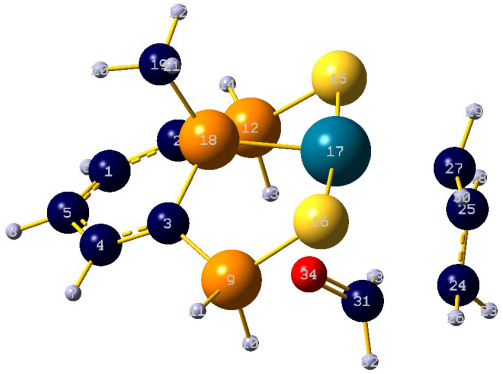
thermodynamics:
Sum of electronic and zero-point Energies=          -2298.609658

Sum of electronic and thermal Enthalpies=           -2298.589308

Sum of electronic and thermal Free Energies=        -2298.659191

  Total free energy in solution:
  with all non electrostatic terms            (a.u.) =   -2298.826569
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{A1A2}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.091638	-1.390075	.932802
2	6	0	-1.905931	-1.457429	.203894
3	6	0	-2.034080	1.282132	.288806
4	6	0	-3.204552	1.057577	1.006811
5	6	0	-3.810046	-.203692	1.157077
6	1	0	-3.452975	-2.285183	1.444514
7	1	0	-3.648431	1.881041	1.571057
8	1	0	-4.754745	-.263210	1.688839
9	15	0	-.833040	2.532336	.609093
10	1	0	-.372520	2.509077	1.940206
11	1	0	-1.432418	3.811635	.536930
12	15	0	-.570037	-2.566426	.493042
13	1	0	-.093810	-2.496395	1.819561
14	1	0	-1.019670	-3.906088	.436703
15	16	0	.927912	-2.330440	-.861648
16	16	0	.681835	2.464823	-.746059
17	46	0	.910745	.079062	-.792937
18	15	0	-1.397980	-.030307	-.749772
19	6	0	-2.425911	-.034285	-2.271080
20	1	0	-3.488506	-.093109	-2.014175
21	1	0	-2.233533	.884604	-2.834370
22	1	0	-2.147510	-.896916	-2.885142
23	1	0	3.991085	-.198582	2.516102
24	6	0	3.366383	.252555	1.745170
25	6	0	3.413322	-.349598	.478087
26	1	0	3.345921	1.342539	1.767625
27	6	0	3.084511	.260977	-.751772
28	1	0	3.600622	-1.424972	.455352
29	1	0	3.361104	-.285461	-1.655561
30	1	0	3.236555	1.338130	-.816346
31	6	0	1.680940	-.207972	2.533658
32	1	0	1.907535	.362518	3.458795
33	1	0	1.904109	-1.288164	2.675827

```
   34          8             0         .653105     .115797    1.858289

HF=-2413.2674159
                     1                     2                     3
                     A                     A                     A
 Frequencies --  -330.9787               34.5479               52.0604
 Red. masses --     9.6020                4.3099                5.4005
 Frc consts  --      .6197                 .0030                 .0086
 IR Inten    --   146.0279                1.0829                1.8444
 Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
   1   6     -.01   -.01    .01       .02   -.02    .01       .12    .02    .15
   2   6     -.01    .00    .02       .00   -.02   -.03       .07    .02    .07
   3   6     -.01   -.01    .01       .05   -.01    .06       .01    .03   -.03
   4   6     -.01    .00    .01       .07   -.02    .08       .05    .02    .05
   5   6     -.01    .00    .01       .05   -.01    .06       .10    .01    .15
   6   1     -.02    .00    .01       .02   -.03   -.01       .18    .04    .21
   7   1     -.02    .00    .01       .10   -.03    .12       .06    .03    .04
   8   1     -.01    .00    .00       .06   -.01    .09       .14    .01    .21
   9  15     -.02    .02   -.03       .05   -.02    .05       .00    .05   -.08
  10   1     -.04    .07   -.01       .02    .03    .06      -.02    .12   -.07
  11   1     -.03    .01    .00       .06   -.01   -.01       .00    .05   -.13
  12  15     -.02   -.02   -.03      -.01   -.03   -.06       .09    .03    .01
  13   1     -.05   -.10   -.01       .01   -.05   -.07       .14   -.01   -.01
  14   1     -.04   -.02   -.03      -.02   -.03   -.07       .09    .03    .00
  15  16      .02   -.01    .02      -.01   -.03   -.07       .02    .03   -.06
  16  16      .01    .01    .02       .06   -.04    .05       .02    .02   -.05
  17  46      .01    .01   -.03       .01   -.04   -.03       .01    .02   -.04
  18  15     -.02    .00    .00       .00    .00    .00       .00    .00    .00
  19   6     -.04    .00    .01      -.04    .08    .03      -.09   -.10    .05
  20   1     -.04    .00   -.02      -.03    .09    .06      -.07   -.13    .12
  21   1     -.02    .00    .01      -.03    .09    .06      -.16   -.12    .00
  22   1     -.02    .00    .01      -.08    .09    .00      -.09   -.11    .08
  23   1      .05   -.11    .13      -.12    .33    .09      -.20   -.18    .13
  24   6      .60    .09   -.17      -.11    .22    .01      -.14   -.13    .12
  25   6      .15    .01    .06      -.06    .06    .09      -.08   -.06    .09
  26   1      .26    .06    .03      -.14    .22   -.12      -.13   -.13    .18
  27   6     -.22   -.04   -.01       .01   -.09   -.01       .00    .01    .10
  28   1      .20    .02    .06      -.06    .06    .23      -.08   -.06    .04
  29   1     -.03   -.06    .05       .04   -.22    .08       .06    .06    .09
  30   1      .07   -.08   -.06       .03   -.10   -.14       .02    .02    .17
  31   6     -.42   -.09    .24      -.11    .24    .04      -.20   -.14    .01
  32   1      .09    .19   -.09      -.17    .39   -.04      -.26   -.15    .03
  33   1     -.05   -.01   -.02      -.04    .27    .21      -.20   -.14    .01
  34   8     -.09   -.02    .14      -.12    .06   -.04      -.16   -.14   -.05

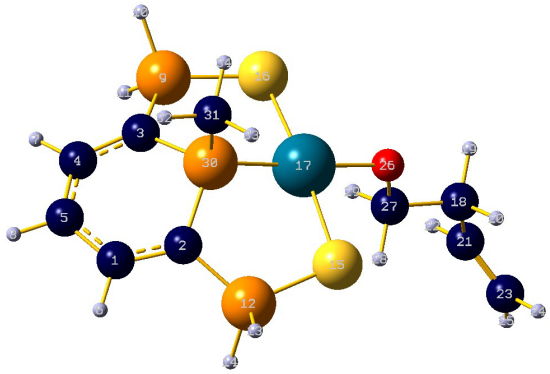
thermodynamics:
Sum of electronic and zero-point Energies=          -2413.019965

Sum of electronic and thermal Enthalpies=           -2412.997781

Sum of electronic and thermal Free Energies=        -2413.069810

 Total free energy in solution:
  with all non electrostatic terms            (a.u.) =   -2413.266563
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.362611	1.504778	1.325278
2	6	0	-2.266940	1.537391	0.467138
3	6	0	-2.522024	-1.215276	0.534584
4	6	0	-3.589100	-0.940157	1.385630
5	6	0	-4.075713	0.345611	1.667525
6	1	0	-3.654237	2.422502	1.839820
7	1	0	-4.041149	-1.762466	1.943528
8	1	0	-4.923160	0.440640	2.338518
9	15	0	-1.585384	-2.709269	0.512998
10	1	0	-2.277627	-3.752178	-0.148790
11	1	0	-1.553272	-3.246890	1.823674
12	15	0	-1.066818	2.827512	0.374452
13	1	0	-1.600581	3.992358	-0.226519
14	1	0	-0.817144	3.329775	1.676344
15	16	0	0.614729	2.275376	-0.622339
16	16	0	0.255969	-2.489770	-0.322454
17	46	0	0.426786	-0.120909	-0.626241
18	6	0	4.649723	-0.325187	-0.058411
19	1	0	4.779383	-1.257892	-0.625605
20	1	0	4.895880	0.502280	-0.734381
21	6	0	5.549356	-0.316670	1.139109
22	1	0	5.425628	-1.149938	1.834862
23	6	0	6.454549	0.622357	1.420337
24	1	0	6.615027	1.473569	0.760506
25	1	0	7.072722	0.575430	2.314014
26	8	0	2.397421	-0.312784	-0.836604
27	6	0	3.159447	-0.225065	0.321721
28	1	0	3.006631	0.730048	0.858877
29	1	0	2.926565	-1.036648	1.039962
30	15	0	-1.816175	0.083665	-0.481443
31	6	0	-2.778287	0.138487	-2.047171
32	1	0	-3.848028	0.249159	-1.841811
33	1	0	-2.429174	0.983553	-2.650570
34	1	0	-2.604918	-0.785140	-2.610375

HF=-2413.306615

		1			2			3		
		A			A			A		
Frequencies --		18.3855			23.2912			31.1476		
Red. masses --		5.0232			4.7543			4.7956		
Frc consts --		0.0010			0.0015			0.0027		
IR Inten --		0.4563			0.3381			0.1961		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.02	-0.03	0.11	0.01	0.11	0.04	-0.04	0.08
2	6	-0.06	-0.01	-0.04	0.05	0.01	0.03	0.01	-0.02	0.03
3	6	0.05	-0.01	0.05	0.04	0.01	0.05	0.01	-0.02	-0.02
4	6	0.05	-0.03	0.05	0.10	0.02	0.12	0.05	-0.04	0.03
5	6	0.00	-0.04	0.01	0.13	0.02	0.16	0.06	-0.05	0.08
6	1	-0.08	-0.01	-0.06	0.15	0.01	0.13	0.06	-0.05	0.11
7	1	0.08	-0.03	0.08	0.13	0.02	0.15	0.07	-0.05	0.03
8	1	0.00	-0.05	0.01	0.17	0.02	0.22	0.09	-0.06	0.12

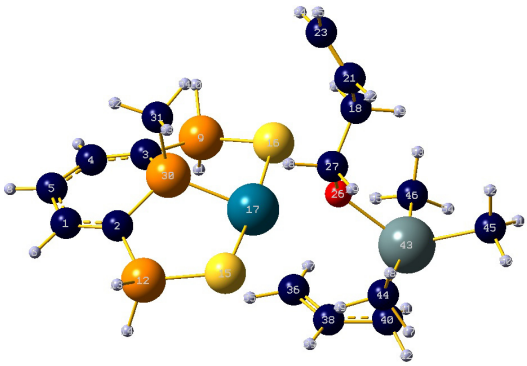
9	15	0.11	0.02	0.10	0.02	0.00	-0.01	-0.01	-0.03	-0.10
10	1	0.10	-0.06	0.23	-0.02	0.01	0.01	0.05	0.06	-0.30
11	1	0.24	0.12	0.14	0.06	-0.01	-0.01	-0.17	-0.18	-0.16
12	15	-0.11	0.04	-0.09	0.05	0.01	-0.04	0.00	-0.01	0.01
13	1	-0.14	-0.03	-0.21	0.03	-0.01	-0.07	-0.04	0.02	0.12
14	1	-0.21	0.16	-0.12	0.07	0.05	-0.06	0.11	-0.08	0.02
15	16	-0.03	0.05	0.04	0.02	-0.02	-0.06	-0.09	0.04	-0.16
16	16	0.03	0.03	-0.07	-0.01	-0.02	-0.08	0.10	0.05	0.15
17	46	0.00	0.05	-0.01	-0.01	-0.01	-0.06	-0.01	0.03	-0.02
18	6	0.00	-0.05	-0.01	-0.03	0.07	0.05	-0.03	-0.12	0.08
19	1	-0.04	-0.01	-0.10	0.05	0.13	-0.02	-0.12	-0.21	0.21
20	1	0.04	0.00	0.07	-0.05	0.15	0.14	0.09	-0.24	-0.03
21	6	-0.01	-0.21	0.00	-0.10	0.02	0.10	-0.06	-0.06	0.10
22	1	-0.06	-0.27	-0.08	-0.07	-0.07	0.01	-0.19	0.05	0.22
23	6	0.03	-0.28	0.09	-0.20	0.07	0.26	0.06	-0.14	-0.01
24	1	0.07	-0.22	0.17	-0.24	0.16	0.36	0.19	-0.26	-0.12
25	1	0.02	-0.39	0.09	-0.25	0.03	0.29	0.03	-0.10	0.02
26	8	0.00	0.10	-0.03	-0.01	0.00	-0.05	0.00	0.02	0.01
27	6	0.00	-0.02	-0.01	-0.06	-0.05	-0.01	-0.02	0.10	0.02
28	1	0.03	-0.06	0.06	-0.13	-0.10	0.06	0.06	0.19	-0.12
29	1	-0.04	-0.07	-0.08	-0.04	-0.11	-0.08	-0.13	0.23	0.13
30	15	0.00	-0.02	0.01	-0.01	0.00	0.01	-0.01	0.00	-0.01
31	6	-0.01	-0.12	0.01	-0.08	0.01	0.06	-0.04	0.04	0.01
32	1	-0.02	-0.16	0.01	-0.07	0.02	0.11	-0.03	0.05	0.03
33	1	-0.05	-0.12	-0.02	-0.11	0.00	0.04	-0.04	0.05	0.02
34	1	0.03	-0.13	0.04	-0.12	0.01	0.05	-0.06	0.05	-0.01

thermodynamics:
Sum of electronic and zero-point Energies= -2413.056661

Sum of electronic and thermal Enthalpies= -2413.033691

Sum of electronic and thermal Free Energies= -2413.111147
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2413.313886

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{A2A1}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.021768	-0.697468	-1.108278
2	6	0	3.666912	-0.455829	-1.324760
3	6	0	3.677938	0.223203	1.351057
4	6	0	5.028773	-0.098564	1.271226
5	6	0	5.705772	-0.410725	0.081824
6	1	0	5.591153	-1.215209	-1.882526
7	1	0	5.600738	-0.193564	2.196224
8	1	0	6.767955	-0.625967	0.132419
9	15	0	2.658670	0.154356	2.787067
10	1	0	3.084496	1.065196	3.780396

11	1	0	2.861608	-1.068942	3.474322
12	15	0	2.662008	-1.199369	-2.563394
13	1	0	2.994190	-0.754332	-3.863980
14	1	0	2.994509	-2.571872	-2.689410
15	16	0	0.684544	-0.853834	-2.241028
16	16	0	0.714891	0.533362	2.331942
17	46	0	0.610876	-0.190582	0.061384
18	6	0	-1.953782	3.081207	-0.158817
19	1	0	-2.934669	2.923092	0.314381
20	1	0	-1.224017	3.193164	0.652799
21	6	0	-1.990560	4.314358	-1.009156
22	1	0	-2.724282	4.315202	-1.818532
23	6	0	-1.196660	5.377339	-0.865984
24	1	0	-0.453133	5.429115	-0.071765
25	1	0	-1.265970	6.239789	-1.524844
26	8	0	-1.577753	0.674353	-0.145173
27	6	0	-1.608623	1.816852	-0.963535
28	1	0	-0.626981	1.963267	-1.440725
29	1	0	-2.334301	1.700107	-1.786531
30	15	0	2.723337	0.508275	-0.141834
31	6	0	2.934349	2.276969	-0.588919
32	1	0	3.997907	2.530042	-0.660389
33	1	0	2.442975	2.464230	-1.549444
34	1	0	2.455265	2.897202	0.175607
35	1	0	0.711484	-2.797380	0.434142
36	6	0	-0.286478	-2.608859	0.823976
37	1	0	-0.371046	-2.463057	1.898406
38	6	0	-1.385572	-2.893701	0.057384
39	1	0	-1.197088	-3.082485	-1.001329
40	6	0	-2.769539	-2.865338	0.453036
41	1	0	-2.961772	-3.039763	1.513012
42	1	0	-3.437671	-3.431214	-0.198365
43	50	0	-3.273866	-0.596842	0.142607
44	6	0	-3.262204	-0.927458	-2.036590
45	6	0	-5.336502	0.150616	0.237004
46	6	0	-2.836026	-0.315766	2.279032
47	1	0	-3.994722	-1.711813	-2.265499
48	1	0	-3.557570	-0.026874	-2.587502
49	1	0	-2.280755	-1.249963	-2.399680
50	1	0	-5.958315	-0.288257	-0.551204
51	1	0	-5.793893	-0.057247	1.210615
52	1	0	-5.343530	1.239464	0.095568
53	1	0	-2.882824	0.750725	2.524914
54	1	0	-3.601894	-0.845665	2.859340
55	1	0	-1.851415	-0.695311	2.563739

HF=-2653.6098931

	1			2			3		
	A			A			A		
Frequencies --	-129.0596			17.8016			19.2228		
Red. masses --	10.6508			4.3887			5.0718		
Frc consts --	0.1045			0.0008			0.0011		
IR Inten --	72.7484			0.2135			0.0845		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.04	0.01	-0.01	0.09	-0.03	0.01	0.00	0.02
2 6	0.02	-0.08	0.02	-0.02	0.08	-0.02	0.00	-0.03	0.01
3 6	0.02	-0.08	0.03	-0.01	0.01	0.00	-0.01	0.09	-0.03
4 6	0.03	-0.04	0.02	-0.01	0.03	-0.01	0.00	0.12	-0.01
5 6	0.02	-0.03	0.01	-0.01	0.07	-0.03	0.00	0.08	0.00
6 1	0.05	-0.01	0.00	-0.01	0.12	-0.05	0.02	-0.02	0.04
7 1	0.05	-0.01	0.01	0.00	0.01	-0.02	0.00	0.18	-0.01
8 1	0.03	0.00	0.01	-0.01	0.08	-0.04	0.01	0.10	0.01
9 15	0.00	0.00	0.02	0.00	-0.04	0.00	0.00	0.14	-0.02
10 1	0.03	0.01	-0.01	0.00	-0.08	0.03	-0.04	0.22	-0.07
11 1	-0.07	0.01	0.06	-0.01	-0.07	-0.04	0.06	0.19	0.06
12 15	0.01	-0.01	-0.01	-0.01	0.09	-0.03	0.01	-0.11	0.04
13 1	0.05	0.02	0.01	-0.05	0.16	-0.02	0.03	-0.20	0.02
14 1	-0.06	-0.02	-0.05	0.04	0.11	-0.09	-0.01	-0.12	0.14

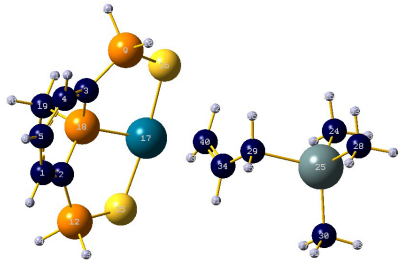
15	16	0.01	0.07	-0.01	-0.02	0.01	0.01	0.01	-0.06	-0.01
16	16	0.02	0.07	-0.03	0.00	-0.02	0.02	-0.02	0.03	-0.03
17	46	-0.03	0.18	-0.06	-0.02	0.00	0.01	0.00	-0.02	-0.01
18	6	0.06	-0.08	0.03	0.17	0.00	-0.03	0.09	-0.01	0.13
19	1	0.07	-0.12	0.03	0.20	0.09	0.07	0.09	0.01	0.15
20	1	0.05	-0.05	0.03	0.26	-0.05	-0.10	0.11	-0.09	0.12
21	6	0.01	-0.08	0.03	0.20	-0.01	-0.04	0.13	0.04	0.20
22	1	0.01	-0.11	0.04	0.12	0.04	0.03	0.11	0.11	0.22
23	6	-0.02	-0.05	0.02	0.32	-0.09	-0.15	0.17	-0.01	0.25
24	1	-0.02	-0.03	0.02	0.41	-0.14	-0.22	0.19	-0.08	0.24
25	1	-0.06	-0.06	0.03	0.34	-0.09	-0.16	0.20	0.04	0.30
26	8	0.17	-0.09	-0.01	-0.02	-0.03	-0.02	0.00	-0.03	0.00
27	6	0.12	-0.06	0.02	-0.02	-0.04	-0.04	0.01	0.01	0.05
28	1	0.11	0.00	0.01	-0.06	-0.13	-0.15	0.00	0.00	0.02
29	1	0.12	-0.10	0.03	-0.11	0.00	0.04	-0.03	0.08	0.08
30	15	0.02	-0.13	0.04	-0.02	0.03	0.02	-0.01	0.01	-0.04
31	6	-0.09	-0.12	0.03	-0.05	0.05	0.06	-0.04	-0.01	-0.13
32	1	-0.10	-0.08	0.04	-0.06	0.06	0.06	-0.05	0.00	-0.15
33	1	-0.10	-0.14	0.03	-0.06	0.07	0.07	-0.05	-0.07	-0.14
34	1	-0.12	-0.14	0.04	-0.06	0.02	0.09	-0.05	0.02	-0.16
35	1	-0.03	-0.13	0.06	0.00	0.00	0.01	-0.01	0.00	0.03
36	6	-0.05	-0.33	0.10	0.00	-0.01	0.01	-0.01	0.00	0.01
37	1	-0.06	-0.28	0.09	0.00	0.00	0.01	-0.03	0.01	0.01
38	6	-0.02	-0.07	0.04	0.00	-0.01	0.02	0.00	0.00	0.00
39	1	-0.02	-0.01	0.03	-0.01	-0.01	0.02	0.01	0.00	0.00
40	6	-0.10	0.13	-0.01	0.00	-0.01	0.02	-0.01	0.00	-0.02
41	1	-0.08	-0.02	-0.02	0.00	-0.01	0.03	-0.02	-0.01	-0.03
42	1	-0.05	0.03	0.01	0.00	-0.03	0.03	0.00	-0.01	-0.03
43	50	-0.02	-0.07	0.02	-0.02	-0.03	0.01	-0.02	-0.01	-0.02
44	6	0.03	0.15	-0.03	-0.04	-0.04	0.01	0.00	0.02	-0.02
45	6	-0.04	-0.11	0.01	-0.02	-0.03	0.02	-0.03	-0.03	-0.03
46	6	0.03	0.19	-0.01	-0.01	0.01	0.00	-0.04	0.00	-0.02
47	1	0.04	0.15	-0.05	-0.04	-0.04	0.02	-0.02	0.05	-0.05
48	1	0.03	0.16	-0.02	-0.04	-0.04	0.01	0.05	0.04	-0.01
49	1	0.03	0.15	-0.05	-0.04	-0.04	0.01	0.00	-0.01	-0.01
50	1	-0.03	-0.10	0.00	-0.02	-0.02	0.01	-0.02	-0.02	-0.05
51	1	-0.04	-0.11	0.01	-0.02	-0.04	0.01	-0.04	-0.04	-0.04
52	1	-0.04	-0.11	0.02	-0.02	-0.03	0.03	-0.04	-0.03	-0.02
53	1	0.09	0.20	-0.05	-0.01	0.01	-0.02	-0.06	0.00	-0.02
54	1	0.03	0.25	0.03	-0.01	0.02	0.01	-0.03	-0.02	-0.02
55	1	0.02	0.15	-0.01	-0.01	0.01	0.00	-0.03	0.01	-0.01

thermodynamics:
Sum of electronic and zero-point Energies= -2653.181382

Sum of electronic and thermal Enthalpies= -2653.144874

Sum of electronic and thermal Free Energies= -2653.252131
  Total free energy in solution:
  with all non electrostatic terms (a.u.) = -2653.598961

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A3.**



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

1	6	0	-4.538699	-0.787956	1.933989
2	6	0	-3.710126	-1.132841	0.865329
3	6	0	-3.408430	1.609551	0.628125
4	6	0	-4.273162	1.638752	1.722672
5	6	0	-4.887769	0.518364	2.292081
6	1	0	-4.898493	-1.584997	2.585204
7	1	0	-4.442071	2.593923	2.220539
8	1	0	-5.542511	0.664164	3.143787
9	15	0	-2.332301	2.912615	0.138776
10	1	0	-1.930786	3.639612	1.282606
11	1	0	-2.971961	3.922271	-0.610928
12	15	0	-2.948102	-2.699912	0.625092
13	1	0	-2.662972	-3.280068	1.882031
14	1	0	-3.808016	-3.669691	0.068372
15	16	0	-1.328947	-2.537514	-0.614643
16	16	0	-0.784189	2.192904	-0.988042
17	46	0	-0.939265	-0.184375	-0.800036
18	15	0	-3.117691	0.101056	-0.279768
19	6	0	-4.127702	0.080264	-1.807328
20	1	0	-5.184471	0.220396	-1.556314
21	1	0	-3.796767	0.882043	-2.475930
22	1	0	-3.993654	-0.876934	-2.322257
23	1	0	6.115051	0.520642	-1.647150
24	6	0	5.023195	0.562454	-1.579431
25	50	0	4.392947	0.027860	0.399878
26	1	0	4.706070	1.579945	-1.828331
27	1	0	4.609876	-0.125419	-2.323246
28	6	0	5.112855	1.387254	1.896628
29	6	0	2.167251	0.282479	0.462217
30	6	0	4.821918	-2.021085	0.874735
31	1	0	6.204877	1.336390	1.954561
32	1	0	4.705970	1.134396	2.880458
33	1	0	4.830746	2.416502	1.655009
34	6	0	1.539673	-0.650187	-0.461665
35	1	0	1.908474	0.084041	1.507264
36	1	0	1.984696	1.332963	0.217967
37	1	0	4.405136	-2.697211	0.121799
38	1	0	5.905135	-2.176792	0.905317
39	1	0	4.413471	-2.291807	1.853435
40	6	0	1.124486	-0.389085	-1.753216
41	1	0	1.465282	-1.684436	-0.121523
42	1	0	1.326664	0.578863	-2.208662
43	1	0	0.929715	-1.210927	-2.439592

HF=-2421.7562288

		1			2			3		
		A			A			A		
Frequencies --		17.3028			21.1265			28.2739		
Red. masses --		6.1384			5.7337			3.5632		
Frc consts --		0.0011			0.0015			0.0017		
IR Inten --		0.4414			0.1428			0.2100		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.18	0.00	0.14	0.04	0.02	0.03	0.02	-0.04	0.01
2	6	0.11	0.00	0.09	-0.01	0.02	-0.01	0.02	-0.02	0.00
3	6	0.04	0.00	0.02	0.11	0.01	0.06	-0.02	-0.01	0.01
4	6	0.11	0.00	0.08	0.15	0.02	0.09	-0.02	-0.04	0.02
5	6	0.18	0.00	0.14	0.12	0.03	0.08	0.01	-0.05	0.01
6	1	0.24	0.00	0.18	0.03	0.02	0.01	0.04	-0.05	0.00
7	1	0.13	0.00	0.08	0.21	0.01	0.13	-0.03	-0.04	0.03
8	1	0.24	0.00	0.19	0.16	0.03	0.11	0.01	-0.06	0.02
9	15	-0.02	0.01	-0.07	0.15	-0.02	0.07	-0.04	0.01	0.02
10	1	-0.01	0.07	-0.11	0.23	-0.08	0.08	-0.07	0.02	0.02
11	1	-0.09	-0.03	-0.08	0.17	0.04	0.13	-0.06	-0.01	0.01
12	15	0.12	0.00	0.06	-0.10	-0.01	-0.08	0.05	-0.01	-0.02
13	1	0.21	0.03	0.04	-0.15	-0.09	-0.11	0.10	0.00	-0.02
14	1	0.09	-0.02	0.13	-0.14	0.07	-0.15	0.06	-0.03	0.01
15	16	0.02	0.02	-0.07	-0.06	-0.04	-0.05	0.01	0.02	-0.06

16	16	-0.04	0.02	-0.10	0.06	-0.05	-0.03	-0.01	0.03	0.04
17	46	0.00	0.02	-0.07	0.00	-0.05	-0.03	0.00	0.03	-0.01
18	15	0.01	-0.01	0.03	0.02	0.03	0.01	0.00	0.00	0.00
19	6	-0.07	-0.06	0.09	-0.01	0.12	0.03	-0.01	-0.01	0.01
20	1	-0.06	-0.09	0.15	0.00	0.16	0.05	-0.01	-0.03	0.02
21	1	-0.14	-0.06	0.06	0.01	0.12	0.05	-0.03	0.00	0.01
22	1	-0.08	-0.07	0.09	-0.07	0.13	0.00	0.00	0.00	0.00
23	1	0.07	0.02	0.15	-0.05	0.05	0.01	-0.02	-0.25	-0.06
24	6	0.06	0.03	0.09	-0.05	0.00	0.00	-0.01	-0.24	-0.06
25	50	-0.05	-0.02	0.04	-0.04	0.05	0.01	0.00	-0.02	0.01
26	1	0.09	0.04	0.11	-0.10	-0.02	-0.04	-0.02	-0.27	-0.16
27	1	0.09	0.06	0.05	-0.01	-0.05	0.02	-0.02	-0.32	0.02
28	6	-0.10	-0.08	0.12	-0.13	0.15	-0.04	0.03	0.14	-0.16
29	6	-0.05	0.01	-0.06	-0.05	-0.05	-0.02	0.00	0.00	0.00
30	6	-0.11	-0.04	0.00	0.07	0.09	0.11	-0.01	0.03	0.24
31	1	-0.11	-0.10	0.18	-0.13	0.24	-0.04	0.02	0.13	-0.15
32	1	-0.16	-0.11	0.10	-0.11	0.16	-0.03	0.02	0.27	-0.13
33	1	-0.08	-0.07	0.15	-0.21	0.12	-0.07	0.04	0.12	-0.28
34	6	-0.02	0.03	-0.10	-0.02	-0.08	-0.01	0.00	0.03	-0.02
35	1	-0.09	-0.01	-0.07	-0.06	-0.05	-0.02	0.00	-0.02	0.00
36	1	-0.03	0.01	-0.05	-0.08	-0.06	-0.03	0.01	0.01	0.03
37	1	-0.10	-0.02	-0.02	0.16	0.04	0.11	-0.02	-0.06	0.31
38	1	-0.11	-0.07	0.03	0.08	0.17	0.17	-0.01	0.02	0.25
39	1	-0.14	-0.06	-0.01	0.04	0.10	0.09	-0.01	0.14	0.27
40	6	-0.01	0.06	-0.10	0.00	-0.11	-0.02	0.00	0.06	-0.01
41	1	-0.02	0.02	-0.13	-0.02	-0.07	0.01	-0.01	0.02	-0.04
42	1	-0.01	0.07	-0.07	0.00	-0.12	-0.04	0.00	0.07	0.01
43	1	0.00	0.08	-0.12	0.01	-0.12	-0.01	0.00	0.08	-0.03

thermodynamics:
Sum of electronic and zero-point Energies= -2421.427691

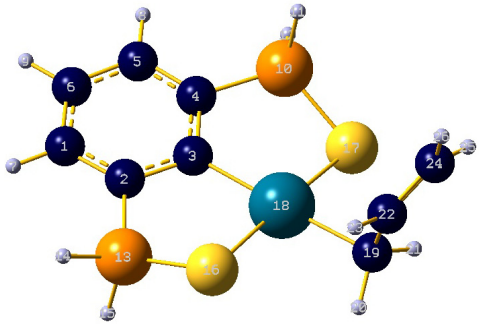
Sum of electronic and thermal Enthalpies= -2421.397724

Sum of electronic and thermal Free Energies= -2421.491647

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2421.785467

S~C~S complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A1.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.546650	-0.734063	0.299998
2	6	0	-2.176473	-0.920740	0.088459
3	6	0	-1.239942	0.130674	0.039882
4	6	0	-1.799323	1.410676	0.226745
5	6	0	-3.159795	1.641962	0.450541

6	6	0	-4.038321	0.558136	0.485298
7	1	0	-4.236486	-1.576249	0.322683
8	1	0	-3.547119	2.648904	0.597206
9	1	0	-5.099076	0.719952	0.653827
10	15	0	-0.546807	2.704290	0.182913
11	1	0	-0.262643	3.068610	1.519861
12	1	0	-1.148674	3.896229	-0.284815
13	15	0	-1.420273	-2.526903	-0.212588
14	1	0	-2.133286	-3.507119	0.516777
15	1	0	-1.750141	-2.908546	-1.534384
16	16	0	0.550771	-2.515413	0.160180
17	16	0	1.067401	2.138443	-0.865863
18	46	0	0.809036	-0.168505	-0.280984
19	6	0	2.881170	-0.448699	-0.538360
20	1	0	2.994430	-1.378348	-1.105337
21	1	0	3.290974	0.387601	-1.112944
22	6	0	3.430059	-0.525440	0.823277
23	1	0	3.294010	-1.477268	1.342533
24	6	0	4.046424	0.466480	1.491107
25	1	0	4.211195	1.441113	1.035136
26	1	0	4.403682	0.333150	2.509106

HF=-1955.7081585

		1			2			3		
		A			A			A		
Frequencies --		28.7704			39.6318			54.5670		
Red. masses --		4.7164			4.3111			5.8837		
Frc consts --		0.0023			0.0040			0.0103		
IR Inten --		1.0960			0.2750			2.0572		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	0.03	0.07	0.04	-0.02	0.13	-0.01	0.02	0.01
2	6	0.00	0.01	0.01	0.03	-0.01	0.06	0.00	0.00	0.06
3	6	0.02	-0.01	-0.01	0.01	0.01	-0.01	0.01	-0.01	0.02
4	6	0.05	0.00	0.04	0.00	0.00	-0.02	0.00	0.00	-0.06
5	6	0.06	0.02	0.11	0.01	-0.01	0.04	-0.01	0.02	-0.13
6	6	0.05	0.03	0.12	0.02	-0.03	0.12	-0.02	0.03	-0.10
7	1	0.00	0.04	0.08	0.05	-0.03	0.18	-0.01	0.02	0.05
8	1	0.09	0.02	0.15	0.00	-0.02	0.04	-0.01	0.03	-0.20
9	1	0.06	0.05	0.17	0.03	-0.04	0.17	-0.02	0.04	-0.15
10	15	0.08	-0.03	0.02	-0.04	0.03	-0.09	-0.02	0.02	-0.02
11	1	0.16	-0.08	0.02	-0.05	0.12	-0.11	-0.16	0.09	-0.01
12	1	0.08	0.00	0.09	-0.07	-0.01	-0.16	-0.02	-0.02	-0.12
13	15	-0.03	0.00	-0.05	0.02	-0.01	0.06	-0.07	-0.06	0.19
14	1	-0.04	-0.01	-0.07	0.07	0.01	0.14	0.07	0.08	0.52
15	1	-0.05	0.05	-0.06	-0.08	-0.05	0.09	-0.38	-0.31	0.33
16	16	-0.02	-0.04	-0.08	0.04	0.01	-0.08	0.01	-0.04	-0.25
17	16	0.01	-0.04	-0.08	-0.01	0.02	-0.05	0.08	0.02	0.15
18	46	0.01	-0.03	-0.02	0.01	0.03	-0.03	0.01	-0.01	0.01
19	6	0.02	-0.03	0.07	0.02	0.05	0.03	0.01	0.00	-0.01
20	1	0.09	-0.09	0.19	0.05	0.12	-0.09	0.03	-0.02	0.03
21	1	0.02	-0.08	0.00	0.06	0.12	0.17	-0.01	-0.02	-0.05
22	6	-0.09	0.16	0.13	-0.08	-0.14	0.06	0.02	0.07	-0.01
23	1	-0.06	0.20	0.22	-0.10	-0.21	-0.09	0.03	0.09	0.04
24	6	-0.24	0.28	0.09	-0.15	-0.22	0.25	0.00	0.11	-0.05
25	1	-0.28	0.25	0.00	-0.13	-0.15	0.40	-0.02	0.09	-0.10
26	1	-0.32	0.42	0.13	-0.23	-0.36	0.26	0.01	0.16	-0.05

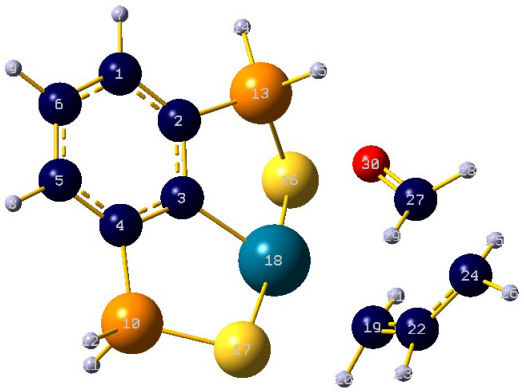
thermodynamics:
Sum of electronic and zero-point Energies= -1955.524857

Sum of electronic and thermal Enthalpies= -1955.507477

Sum of electronic and thermal Free Energies= -1955.570881

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1955.717128

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{A1A2}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054094	-0.642031	0.580931
2	6	0	0.203622	0.246446	1.625344
3	6	0	1.500767	0.683394	1.956350
4	6	0	2.534206	0.168426	1.152922
5	6	0	2.308893	-0.712078	0.087760
6	6	0	1.006369	-1.117442	-0.195346
7	1	0	-1.068227	-0.970083	0.361618
8	1	0	3.132499	-1.086068	-0.517153
9	1	0	0.816002	-1.804161	-1.015028
10	15	0	4.129668	0.773605	1.692927
11	1	0	4.476728	1.889751	0.898006
12	1	0	5.125965	-0.151614	1.303462
13	15	0	-1.013623	0.984222	2.727423
14	1	0	-2.264420	0.956812	2.066620
15	1	0	-1.182894	0.149493	3.846914
16	16	0	-0.390033	2.836146	3.196165
17	16	0	4.098567	1.156749	3.664567
18	46	0	1.800692	1.882921	3.579140
19	6	0	2.070299	3.254310	5.297627
20	1	0	2.847083	3.897964	4.882029
21	1	0	1.101075	3.737067	5.413144
22	6	0	2.462931	2.365408	6.318853
23	1	0	3.526963	2.118793	6.368295
24	6	0	1.615224	1.642813	7.172951
25	1	0	0.611588	2.037819	7.325592
26	1	0	2.074277	1.224653	8.068712
27	6	0	1.156322	0.032031	6.248803
28	1	0	0.659678	-0.419917	7.134034
29	1	0	2.184352	-0.364275	6.124710
30	8	0	0.453511	0.271675	5.219194

HF=-2070.1504982

	1			2			3		
	A			A			A		
Frequencies --	-320.5363			39.6043			48.8608		
Red. masses --	9.8927			6.2474			4.5630		
Frc consts --	0.5989			0.0058			0.0064		
IR Inten --	165.3081			0.4990			0.8139		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.01	-0.02	-0.02	-0.01	-0.09	0.15	0.00	0.02	-0.02
2 6	0.00	-0.03	-0.02	0.00	0.01	0.06	-0.01	0.02	-0.03
3 6	-0.01	-0.05	0.00	0.00	0.03	0.02	-0.01	0.01	0.00
4 6	-0.01	-0.03	-0.01	-0.01	-0.04	0.05	0.00	-0.02	0.04
5 6	0.00	-0.01	-0.02	-0.02	-0.14	0.13	0.02	-0.04	0.05
6 6	0.00	-0.01	-0.02	-0.02	-0.17	0.19	0.02	-0.01	0.01
7 1	-0.01	-0.02	-0.04	-0.01	-0.11	0.19	0.00	0.03	-0.05

8	1	-0.01	0.00	-0.04	-0.02	-0.20	0.16	0.03	-0.06	0.08
9	1	0.00	-0.01	-0.03	-0.03	-0.25	0.26	0.03	-0.02	0.02
10	15	-0.01	-0.01	0.01	0.00	-0.01	-0.03	0.00	-0.06	0.09
11	1	-0.02	-0.01	0.01	-0.01	-0.06	-0.11	0.06	-0.09	0.07
12	1	0.02	0.02	0.01	-0.01	-0.03	0.02	-0.02	-0.10	0.14
13	15	-0.02	0.02	-0.06	-0.02	0.07	0.01	-0.01	0.04	-0.05
14	1	0.00	0.07	-0.10	0.02	0.12	-0.06	-0.02	0.00	-0.03
15	1	-0.25	-0.04	-0.16	-0.12	0.08	0.00	0.01	0.06	-0.03
16	16	0.00	-0.02	0.03	0.03	0.05	0.02	-0.03	0.06	-0.08
17	16	0.00	0.01	0.01	0.04	0.13	-0.05	-0.06	-0.01	0.07
18	46	0.01	0.05	-0.01	0.03	0.07	-0.01	-0.05	0.01	0.00
19	6	-0.01	-0.14	-0.17	-0.01	-0.04	0.07	-0.10	0.00	0.02
20	1	0.03	-0.03	0.06	0.01	-0.01	0.16	-0.20	0.10	-0.02
21	1	0.10	0.03	0.03	-0.01	-0.04	0.07	-0.15	-0.12	0.10
22	6	0.04	0.04	0.14	-0.06	-0.13	0.00	0.08	0.02	-0.02
23	1	0.04	0.03	0.13	-0.07	-0.15	0.02	0.11	0.15	-0.11
24	6	0.19	0.48	0.36	-0.09	-0.20	-0.08	0.23	-0.10	0.01
25	1	0.00	0.05	0.11	-0.10	-0.21	-0.09	0.20	-0.21	0.12
26	1	0.08	0.00	0.17	-0.12	-0.25	-0.09	0.34	-0.13	-0.06
27	6	-0.12	-0.42	-0.22	-0.04	-0.16	-0.16	0.25	-0.06	-0.12
28	1	0.00	0.10	0.09	-0.03	-0.22	-0.18	0.37	-0.18	-0.11
29	1	0.03	0.02	-0.15	-0.04	-0.13	-0.18	0.27	0.03	-0.26
30	8	-0.08	-0.17	0.05	-0.06	-0.13	-0.15	0.14	0.01	-0.02

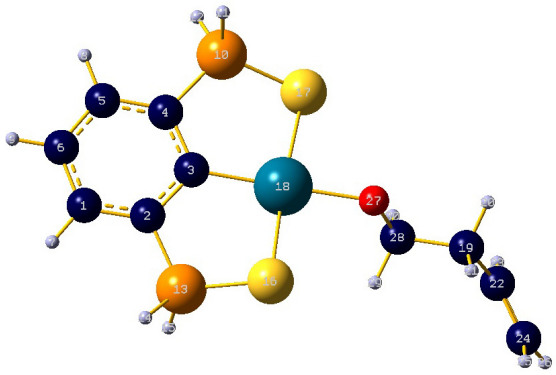
thermodynamics:
Sum of electronic and zero-point Energies= -2069.936100

Sum of electronic and thermal Enthalpies= -2069.916866

Sum of electronic and thermal Free Energies= -2069.983101

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2070.158662

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.693235	1.657164	0.528864
2	6	0	-2.340377	1.429654	0.258596
3	6	0	-1.784979	0.143073	0.063738
4	6	0	-2.721909	-0.911268	0.171808
5	6	0	-4.080441	-0.715855	0.439470
6	6	0	-4.569848	0.577079	0.617326
7	1	0	-4.073906	2.667026	0.671701
8	1	0	-4.763828	-1.560048	0.513503
9	1	0	-5.622883	0.741066	0.825712
10	15	0	-2.005203	-2.540234	-0.086114
11	1	0	-2.463021	-3.014929	-1.338031

12	1	0	-2.665828	-3.440738	0.781524
13	15	0	-1.125275	2.752748	0.172943
14	1	0	-1.748971	3.881044	-0.407481
15	1	0	-0.922989	3.224254	1.491716
16	16	0	0.541045	2.148672	-0.762745
17	16	0	-0.009986	-2.498184	0.100145
18	46	0	0.186381	-0.158213	-0.299045
19	6	0	4.444665	-0.424481	-0.244343
20	1	0	4.496944	-1.420914	-0.705994
21	1	0	4.603336	0.309896	-1.043170
22	6	0	5.492929	-0.288728	0.816498
23	1	0	5.452194	-1.023358	1.624238
24	6	0	6.437771	0.652649	0.855466
25	1	0	6.519616	1.408306	0.075691
26	1	0	7.167252	0.702212	1.660733
27	8	0	2.113078	-0.473139	-0.730421
28	6	0	3.014165	-0.253459	0.303566
29	1	0	2.933307	0.762270	0.736881
30	1	0	2.878431	-0.963673	1.145661

HF=-2070.19125

		1			2			3		
		A			A			A		
Frequencies --		18.9185			26.4916			35.8368		
Red. masses --		5.6241			5.1095			5.4131		
Frc consts --		0.0012			0.0021			0.0041		
IR Inten --		1.2309			1.1782			1.4798		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.04	-0.05	0.02	0.07	0.04	0.12	0.01	-0.02	0.10
2	6	-0.04	-0.02	-0.01	0.05	0.01	0.04	0.00	-0.01	0.05
3	6	0.00	0.00	0.01	0.02	0.00	0.01	0.00	0.00	0.00
4	6	0.04	-0.03	0.07	0.01	0.02	0.06	0.00	0.00	-0.04
5	6	0.04	-0.07	0.11	0.03	0.04	0.14	0.01	-0.02	0.00
6	6	0.00	-0.08	0.08	0.06	0.05	0.18	0.02	-0.02	0.08
7	1	-0.07	-0.06	0.00	0.10	0.04	0.15	0.01	-0.02	0.15
8	1	0.07	-0.09	0.16	0.02	0.05	0.19	0.01	-0.02	-0.02
9	1	0.00	-0.11	0.11	0.08	0.07	0.24	0.02	-0.03	0.12
10	15	0.07	-0.02	0.10	-0.04	0.01	0.02	0.05	0.04	-0.16
11	1	-0.02	-0.11	0.17	-0.12	0.01	0.05	0.33	0.27	-0.35
12	1	0.17	0.01	0.21	-0.01	0.02	0.06	-0.12	-0.12	-0.46
13	15	-0.09	0.03	-0.08	0.07	-0.01	-0.02	0.02	-0.02	0.03
14	1	-0.14	-0.03	-0.14	0.06	0.00	-0.01	-0.01	0.02	0.13
15	1	-0.13	0.11	-0.10	0.12	0.01	-0.03	0.13	-0.09	0.03
16	16	-0.05	0.06	-0.03	0.03	-0.04	-0.08	-0.06	-0.01	-0.12
17	16	0.08	0.04	-0.06	-0.03	-0.03	-0.10	0.01	0.03	0.27
18	46	0.00	0.05	-0.04	0.00	-0.03	-0.06	0.00	0.00	-0.02
19	6	-0.01	-0.06	0.02	-0.01	0.09	0.03	0.00	0.05	-0.04
20	1	-0.06	-0.03	-0.05	0.09	0.14	-0.05	0.00	0.10	-0.16
21	1	0.07	-0.01	0.08	-0.03	0.18	0.11	0.00	0.14	0.04
22	6	-0.04	-0.21	0.07	-0.07	0.08	0.10	-0.01	-0.07	-0.02
23	1	-0.12	-0.27	0.01	-0.03	-0.01	0.01	-0.01	-0.17	-0.11
24	6	0.02	-0.28	0.18	-0.17	0.18	0.25	-0.02	-0.07	0.10
25	1	0.11	-0.22	0.25	-0.22	0.28	0.33	-0.02	0.03	0.20
26	1	-0.01	-0.40	0.22	-0.22	0.17	0.29	-0.03	-0.16	0.11
27	8	0.01	0.11	-0.07	0.00	-0.04	-0.05	-0.01	0.05	-0.05
28	6	-0.02	-0.01	-0.02	-0.04	-0.06	-0.01	-0.01	-0.03	-0.03
29	1	0.02	-0.03	0.04	-0.13	-0.10	0.08	-0.02	-0.07	0.06
30	1	-0.09	-0.05	-0.07	-0.02	-0.14	-0.07	0.01	-0.10	-0.09

thermodynamics:
Sum of electronic and zero-point Energies= -2069.974574

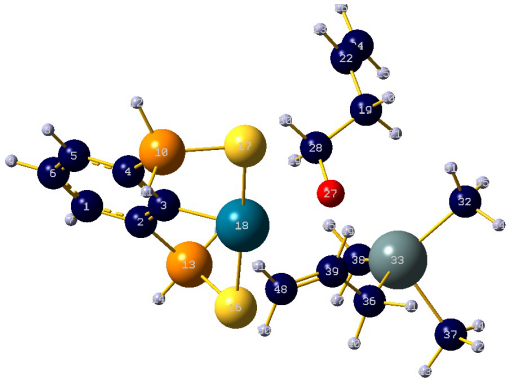
Sum of electronic and thermal Enthalpies= -2069.954613

Sum of electronic and thermal Free Energies= -2070.025666

Total free energy in solution:

```
 with all non electrostatic terms            (a.u.) =   -2070.206336
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{A2A1}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.126820	0.550267	2.357486
2	6	0	2.921780	0.122272	1.796274
3	6	0	2.751236	-0.094177	0.408189
4	6	0	3.898972	0.157138	-0.378849
5	6	0	5.117544	0.577137	0.161192
6	6	0	5.232060	0.774963	1.536549
7	1	0	4.212873	0.711412	3.429941
8	1	0	5.977906	0.753936	-0.480674
9	1	0	6.173252	1.105257	1.965033
10	15	0	3.565021	-0.119198	-2.111758
11	1	0	3.935140	-1.445128	-2.431468
12	1	0	4.487744	0.624160	-2.881956
13	15	0	1.413772	-0.233371	2.692855
14	1	0	1.738828	-0.558902	4.029068
15	1	0	0.676376	0.959290	2.843751
16	16	0	0.449895	-1.681838	1.695793
17	16	0	1.637823	0.313110	-2.468181
18	46	0	0.991512	-0.624488	-0.370028
19	6	0	-1.694255	2.971019	-0.723292
20	1	0	-1.943255	2.816770	-1.782245
21	1	0	-2.618247	2.832318	-0.150552
22	6	0	-1.161581	4.356263	-0.519467
23	1	0	-0.300543	4.630148	-1.134393
24	6	0	-1.630143	5.248458	0.355491
25	1	0	-2.485466	5.026508	0.991741
26	1	0	-1.186339	6.235681	0.463420
27	8	0	-1.034967	0.589031	-0.619292
28	6	0	-0.658352	1.899140	-0.326312
29	1	0	-0.438254	2.046382	0.752360
30	1	0	0.280164	2.154649	-0.851482
31	1	0	-3.527493	1.092125	-2.144388
32	6	0	-4.157393	0.740250	-1.323798
33	50	0	-3.017740	-0.366967	0.148590
34	1	0	-4.930648	0.075813	-1.726396
35	1	0	-4.662343	1.604930	-0.878658
36	6	0	-2.163141	-2.181640	-0.821070
37	6	0	-4.683037	-1.588316	0.970827
38	6	0	-2.565091	0.519538	2.086155
39	6	0	-0.967943	-2.076202	-1.663488
40	1	0	-2.069874	-2.966145	-0.060953
41	1	0	-3.029290	-2.432121	-1.449530
42	1	0	-5.167728	-2.197150	0.196129
43	1	0	-4.337106	-2.269950	1.759448
44	1	0	-5.453391	-0.942605	1.412918
45	1	0	-1.766702	1.266139	2.082892

46	1	0	-3.479960	0.986595	2.470114
47	1	0	-2.298633	-0.292398	2.772401
48	6	0	0.202281	-2.752323	-1.501818
49	1	0	-1.045958	-1.410778	-2.524014
50	1	0	0.320155	-3.503390	-0.722832
51	1	0	0.992048	-2.695518	-2.246239

HF=-2310.5008412

	1			2			3		
	A			A			A		
Frequencies --	-100.6193			10.3674			28.4818		
Red. masses --	15.1579			5.2663			4.4924		
Frc consts --	0.0904			0.0003			0.0021		
IR Inten --	10.4846			0.1361			0.2098		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.08	-0.09	-0.04	0.03	0.10	-0.05	-0.06	0.01	0.03
2 6	0.10	-0.18	-0.02	0.02	0.07	-0.03	-0.06	0.02	0.00
3 6	0.10	-0.24	-0.01	0.01	0.02	-0.02	-0.02	0.00	0.00
4 6	0.08	-0.18	-0.03	0.00	0.01	-0.04	0.01	-0.04	0.03
5 6	0.06	-0.09	-0.05	0.00	0.04	-0.07	0.00	-0.05	0.05
6 6	0.06	-0.05	-0.06	0.01	0.09	-0.07	-0.04	-0.03	0.05
7 1	0.07	-0.03	-0.05	0.04	0.14	-0.06	-0.09	0.02	0.03
8 1	0.03	-0.03	-0.07	-0.01	0.03	-0.08	0.02	-0.08	0.08
9 1	0.04	0.02	-0.07	0.01	0.11	-0.10	-0.04	-0.03	0.08
10 15	0.01	-0.07	-0.03	-0.02	-0.04	-0.03	0.05	-0.07	0.02
11 1	-0.12	-0.09	-0.11	-0.01	-0.05	0.01	0.03	-0.09	0.07
12 1	0.05	-0.11	-0.02	-0.04	-0.06	-0.06	0.09	-0.11	0.03
13 15	0.08	-0.04	0.02	0.04	0.08	0.01	-0.08	0.05	-0.03
14 1	0.10	-0.11	0.00	0.06	0.11	0.01	-0.12	0.05	-0.02
15 1	0.25	0.05	0.09	0.04	0.08	-0.01	-0.07	0.06	-0.06
16 16	-0.13	0.13	0.02	0.03	0.05	0.06	-0.07	0.05	-0.04
17 16	0.03	0.10	0.04	-0.03	-0.07	-0.02	0.07	-0.03	-0.04
18 46	-0.06	0.25	0.08	0.01	-0.02	0.02	-0.01	0.01	-0.04
19 6	0.03	-0.07	0.00	0.01	-0.01	0.16	-0.09	-0.01	0.09
20 1	0.01	-0.06	0.00	-0.05	0.05	0.17	-0.24	0.03	0.12
21 1	0.06	-0.11	0.03	0.04	-0.03	0.21	-0.01	-0.07	0.21
22 6	0.00	-0.06	0.00	0.03	-0.02	0.21	-0.12	0.00	0.08
23 1	-0.01	-0.04	-0.02	0.00	0.00	0.18	-0.21	0.06	-0.02
24 6	-0.01	-0.07	0.00	0.08	-0.06	0.27	-0.04	-0.05	0.18
25 1	0.00	-0.09	0.01	0.11	-0.09	0.31	0.04	-0.11	0.27
26 1	-0.04	-0.05	-0.02	0.10	-0.07	0.30	-0.07	-0.04	0.16
27 8	0.13	-0.05	-0.09	0.00	-0.02	0.00	-0.01	0.01	-0.08
28 6	0.09	-0.04	-0.05	0.03	-0.04	0.04	0.00	0.01	-0.11
29 1	0.10	-0.07	-0.05	0.10	-0.09	0.04	0.17	-0.01	-0.14
30 1	0.06	0.03	-0.06	0.00	-0.01	0.00	-0.09	0.05	-0.24
31 1	0.09	-0.04	-0.03	0.12	-0.05	-0.11	-0.04	-0.14	-0.05
32 6	0.07	-0.03	-0.04	0.07	0.00	-0.13	-0.02	-0.07	0.01
33 50	-0.02	-0.08	-0.02	-0.03	0.00	-0.05	0.04	0.01	0.02
34 1	0.06	-0.01	-0.06	0.06	0.02	-0.14	-0.05	-0.08	0.09
35 1	0.08	-0.02	-0.05	0.09	0.04	-0.18	0.02	-0.03	-0.03
36 6	-0.01	-0.08	0.06	-0.01	-0.03	0.03	0.03	-0.01	0.02
37 6	-0.07	0.04	0.01	-0.09	0.05	-0.11	0.11	0.00	0.13
38 6	0.04	0.00	-0.07	-0.07	0.00	-0.04	0.05	0.13	-0.04
39 6	-0.04	-0.15	-0.04	0.01	-0.06	0.05	0.00	0.00	-0.01
40 1	0.06	-0.03	0.10	-0.02	0.00	0.06	0.05	0.00	0.03
41 1	-0.03	-0.20	0.13	0.01	-0.05	0.02	0.01	-0.01	0.05
42 1	-0.10	0.04	0.02	-0.07	0.05	-0.12	0.08	-0.04	0.17
43 1	-0.10	0.03	0.02	-0.14	0.06	-0.08	0.16	0.02	0.14
44 1	-0.05	0.07	0.00	-0.10	0.08	-0.15	0.11	-0.01	0.15
45 1	0.13	-0.10	-0.09	-0.08	0.01	-0.03	0.08	0.10	-0.08
46 1	0.08	0.13	-0.14	-0.08	-0.02	-0.05	0.07	0.20	-0.09
47 1	-0.08	0.01	-0.02	-0.06	0.00	-0.05	0.01	0.18	0.03
48 6	-0.09	-0.19	-0.11	0.01	-0.05	0.10	0.01	0.01	-0.04
49 1	-0.06	-0.13	-0.02	0.03	-0.09	0.02	-0.03	-0.01	-0.01
50 1	-0.02	-0.13	-0.05	-0.01	-0.03	0.13	0.04	0.01	-0.04
51 1	-0.05	-0.12	-0.06	0.02	-0.08	0.11	-0.01	0.01	-0.06

thermodynamics:

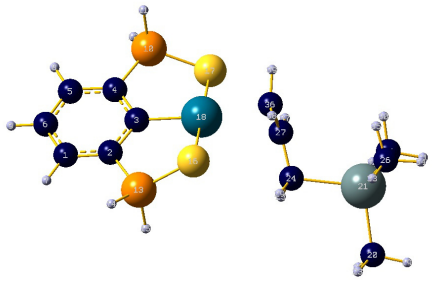
Sum of electronic and zero-point Energies= -2310.104263

Sum of electronic and thermal Enthalpies= -2310.071360

Sum of electronic and thermal Free Energies= -2310.169469

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2310.497378

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **A3.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.098761	.246338	-.170283
2	6	0	.039668	.282842	1.227552
3	6	0	1.169366	.103456	2.055215
4	6	0	2.380827	-.105795	1.361362
5	6	0	2.469150	-.136609	-.035407
6	6	0	1.320936	.036224	-.803762
7	1	0	-.797386	.385755	-.770576
8	1	0	3.423830	-.297934	-.530853
9	1	0	1.378448	.010055	-1.887259
10	15	0	3.803393	-.311802	2.429718
11	1	0	4.539761	.891116	2.448158
12	1	0	4.713337	-1.207643	1.834028
13	15	0	-1.479052	.568226	2.133070
14	1	0	-2.315282	1.420428	1.384870
15	1	0	-2.226779	-.628065	2.163601
16	16	0	-1.017867	1.299007	3.953705
17	16	0	3.171986	-.913046	4.247173
18	46	0	1.061985	.165349	4.092221
19	1	0	-2.904210	-3.079361	9.976346
20	6	0	-2.678316	-2.812802	8.938888
21	50	0	-.849789	-1.693629	8.848311
22	1	0	-2.596768	-3.736732	8.358312
23	1	0	-3.513565	-2.224681	8.546859
24	6	0	-.581349	-1.278658	6.658398
25	6	0	.850406	-2.831434	9.497057
26	6	0	-.983486	.213732	9.819838
27	6	0	.732111	-.694984	6.438958
28	1	0	-.694185	-2.262790	6.192292
29	1	0	-1.409356	-.622425	6.376536
30	1	0	1.764549	-2.231015	9.458424
31	1	0	.705628	-3.160052	10.531217
32	1	0	.988493	-3.722048	8.875915
33	1	0	-1.859942	.768575	9.471335
34	1	0	-1.075580	.075724	10.901964
35	1	0	-.089072	.814873	9.629582
36	6	0	1.042738	.647063	6.311322
37	1	0	1.570697	-1.392735	6.483149
38	1	0	.272272	1.401291	6.458697
39	1	0	2.069989	.981695	6.435414

HF=-2078.6413313

1 2 3

		A			A			A	
Frequencies --		15.1570			21.4216			27.4464	
Red. masses --		3.7335			5.2426			5.9995	
Frc consts --		.0005			.0014			.0027	
IR Inten --		.1437			.8394			.2942	
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.01	.02	-.01	.07	.17	-.05	.10	-.01	-.06
2	6	.00	-.01	-.01	.04	.08	-.05	.05	.01	-.06
3	6	.01	.01	-.01	.02	.03	-.03	.01	.00	-.01
4	6	.02	.06	-.01	.03	.06	-.01	.03	-.05	.04
5	6	.02	.10	-.01	.07	.15	-.01	.08	-.08	.04
6	6	.02	.07	-.01	.09	.20	-.03	.11	-.06	-.01
7	1	.01	.01	-.01	.09	.21	-.06	.12	.00	-.09
8	1	.03	.14	-.01	.08	.17	.01	.09	-.11	.08
9	1	.03	.10	-.01	.12	.27	-.03	.15	-.08	.00
10	15	.02	.09	.00	.00	-.01	.02	-.01	-.06	.08
11	1	-.02	.11	.03	.02	-.02	.10	.03	-.09	.07
12	1	.05	.13	-.02	.01	.01	-.01	-.02	-.11	.14
13	15	-.01	-.07	-.01	.02	.04	-.07	.01	.07	-.13
14	1	-.03	-.09	.00	.03	.07	-.04	.08	.10	-.16
15	1	.03	-.10	-.02	.02	.04	-.14	-.03	.09	-.17
16	16	-.03	-.08	.00	-.02	-.05	-.02	-.05	.04	-.10
17	16	.03	.02	-.02	-.05	-.10	-.03	-.08	.01	.08
18	46	.00	-.02	-.01	-.03	-.06	-.03	-.06	.04	-.02
19	1	-.12	.20	.05	.12	-.04	.17	.07	-.01	.09
20	6	-.12	.20	.05	.07	-.08	.15	.01	.04	.09
21	50	-.01	.01	.01	.01	.02	.05	.05	-.03	.03
22	1	-.23	.21	.03	.12	-.11	.20	-.07	.07	.03
23	1	-.07	.30	.09	.03	-.15	.14	.01	.09	.18
24	6	.01	-.06	.00	-.06	-.06	.02	-.06	.04	.03
25	6	-.12	-.15	.02	.09	.16	.06	.04	-.13	-.13
26	6	.22	.06	-.04	-.07	.07	-.05	.19	-.07	.12
27	6	.00	-.05	-.01	-.05	-.09	-.01	-.08	.08	.00
28	1	.01	-.07	.02	-.10	-.06	.05	-.04	.04	.01
29	1	.00	-.07	-.01	-.06	-.04	.03	-.09	.02	.06
30	1	-.06	-.25	.01	.06	.21	-.01	.06	-.16	-.15
31	1	-.15	-.12	.03	.15	.21	.08	.09	-.17	-.13
32	1	-.21	-.18	.04	.12	.13	.10	-.03	-.10	-.17
33	1	.21	.10	.03	-.16	-.04	.01	.21	.00	.17
34	1	.33	.11	-.03	.07	.13	-.03	.21	-.11	.12
35	1	.24	-.01	-.17	-.15	.14	-.19	.22	-.11	.12
36	6	.00	-.05	.00	-.03	-.10	-.02	-.13	.09	-.03
37	1	.01	-.05	-.01	-.07	-.11	-.03	-.06	.11	.02
38	1	-.01	-.06	.00	-.01	-.08	-.01	-.15	.06	-.05
39	1	-.01	-.05	.00	-.02	-.12	-.03	-.14	.13	-.03

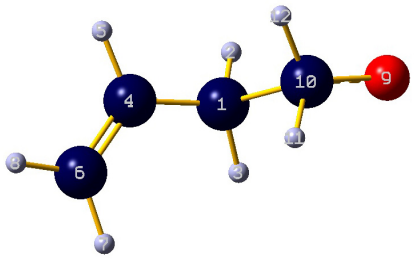
thermodynamics:
Sum of electronic and zero-point Energies= -2078.345736

Sum of electronic and thermal Enthalpies= -2078.318890

Sum of electronic and thermal Free Energies= -2078.406269

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2078.676795

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **allylalcoolate.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.017655	0.039665	0.110581
2	1	0	-0.087690	-0.065856	1.198262
3	1	0	1.088448	0.021017	-0.131666
4	6	0	-0.641419	1.262869	-0.386640
5	1	0	-1.617229	1.488453	0.057694
6	6	0	-0.248716	2.036426	-1.415891
7	1	0	0.702446	1.866640	-1.920525
8	1	0	-0.861317	2.853832	-1.796168
9	8	0	-0.068910	-2.416258	0.036308
10	6	0	-0.595317	-1.355864	-0.495573
11	1	0	-0.447832	-1.189394	-1.618086
12	1	0	-1.728512	-1.208330	-0.371826

HF=-231.7069282

	1			2			3		
	A			A			A		
Frequencies --	82.4247			127.1333			254.1590		
Red. masses --	2.5159			2.8702			1.9197		
Frc consts --	0.0101			0.0273			0.0731		
IR Inten --	4.0731			3.1292			1.5027		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	0.04	0.16	-0.14	0.01	0.09	0.13	0.05	0.09
2 1	-0.13	-0.04	0.14	-0.15	0.09	0.10	0.14	0.11	0.09
3 1	0.03	0.04	0.28	-0.14	-0.08	0.09	0.12	0.11	0.05
4 6	0.05	0.04	0.13	-0.02	0.04	0.00	-0.04	-0.11	-0.06
5 1	0.16	0.23	0.27	-0.02	0.18	-0.07	-0.24	-0.43	-0.35
6 6	-0.07	-0.20	-0.11	0.12	-0.08	-0.05	-0.01	-0.05	0.01
7 1	-0.20	-0.42	-0.27	0.13	-0.24	0.02	0.19	0.25	0.29
8 1	-0.05	-0.20	-0.14	0.24	-0.04	-0.15	-0.18	-0.28	-0.22
9 8	-0.05	0.03	-0.08	0.18	0.03	-0.16	-0.07	-0.01	-0.09
10 6	0.08	0.09	-0.07	-0.15	0.00	0.12	0.02	0.11	0.08
11 1	0.32	0.22	-0.02	-0.52	0.14	0.09	-0.08	0.19	0.07
12 1	0.06	0.10	-0.29	-0.13	-0.16	0.50	0.04	0.22	0.20

thermodynamics:

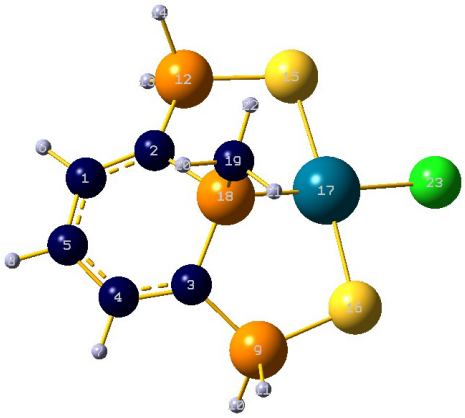
Sum of electronic and zero-point Energies= -231.609059
Sum of electronic and thermal Enthalpies= -231.602120
Sum of electronic and thermal Free Energies= -231.638425

Total free energy in solution:
with all non electrostatic terms (a.u.) = -231.792499

III. Lewis acid mechanism

S~P~*S* complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B0.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.159964	-1.227384	-0.553415
2	6	0	1.855616	-1.385002	-0.092224
3	6	0	1.855650	1.384968	-0.092194
4	6	0	3.159991	1.227327	-0.553394
5	6	0	3.828552	-0.000036	-0.666272
6	1	0	3.689680	-2.105282	-0.927102
7	1	0	3.689726	2.105218	-0.927070
8	1	0	4.849834	-0.000044	-1.032086
9	15	0	0.826284	2.794248	-0.339849
10	1	0	1.092026	3.340698	-1.619868
11	1	0	1.218373	3.884987	0.471303
12	15	0	0.826212	-2.794249	-0.339907
13	1	0	1.091868	-3.340630	-1.619974
14	1	0	1.218322	-3.885044	0.471159
15	16	0	-1.139674	-2.383118	-0.002379
16	16	0	-1.139633	2.383138	-0.002461
17	46	0	-1.192427	0.000015	0.055069
18	15	0	0.966951	-0.000015	0.613981
19	6	0	1.253306	-0.000032	2.427043
20	1	0	2.326913	-0.000035	2.643486
21	1	0	0.786337	0.888552	2.865143
22	1	0	0.786332	-0.888613	2.865142
23	17	0	-3.494061	0.000023	-0.439793

HF=-2641.755403

	1			2			3		
	A			A			A		
Frequencies --	24.9568			36.3834			55.0292		
Red. masses --	7.0478			4.3171			13.1789		
Frc consts --	0.0026			0.0034			0.0235		
IR Inten --	0.0592			6.1374			0.8834		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.02	0.06	0.05	0.00	0.13	-0.06	0.00	-0.10
2 6	0.01	-0.01	0.06	0.00	0.01	-0.01	-0.03	0.00	-0.02
3 6	-0.01	-0.01	-0.06	0.00	-0.01	-0.01	-0.03	0.00	-0.02
4 6	-0.01	-0.02	-0.06	0.05	0.00	0.13	-0.06	0.00	-0.10
5 6	0.00	-0.02	0.00	0.07	0.00	0.23	-0.06	0.00	-0.13
6 1	0.02	-0.03	0.11	0.09	0.01	0.17	-0.09	0.00	-0.15
7 1	-0.02	-0.03	-0.11	0.09	-0.01	0.17	-0.09	0.00	-0.15
8 1	0.00	-0.03	0.00	0.12	0.00	0.36	-0.08	0.00	-0.19
9 15	-0.04	-0.04	-0.14	-0.02	-0.05	-0.17	-0.06	-0.03	-0.05
10 1	-0.25	-0.24	-0.27	-0.14	-0.24	-0.28	-0.23	-0.17	-0.14
11 1	0.09	0.08	-0.37	0.04	0.08	-0.37	0.03	0.06	-0.22
12 15	0.04	-0.04	0.14	-0.02	0.05	-0.17	-0.06	0.03	-0.05
13 1	0.25	-0.24	0.27	-0.14	0.24	-0.28	-0.23	0.17	-0.14
14 1	-0.09	0.08	0.37	0.04	-0.08	-0.37	0.03	-0.06	-0.22

15	16	-0.02	0.02	-0.26	0.01	0.00	0.04	-0.01	-0.01	0.25
16	16	0.02	0.02	0.26	0.01	0.00	0.04	-0.01	0.01	0.25
17	46	0.00	0.00	0.00	-0.01	0.00	0.01	0.01	0.00	0.04
18	15	0.00	0.02	0.00	0.00	0.00	-0.01	0.02	0.00	0.06
19	6	0.00	0.11	0.00	0.03	0.00	-0.01	0.18	0.00	0.03
20	1	0.00	0.13	0.00	0.04	0.00	-0.04	0.20	0.00	-0.07
21	1	-0.01	0.13	-0.05	0.04	0.00	-0.01	0.23	0.00	0.08
22	1	0.01	0.13	0.05	0.04	0.00	-0.01	0.23	0.00	0.08
23	17	0.00	0.00	0.00	-0.02	0.00	0.06	0.12	0.00	-0.42

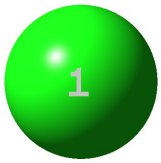
thermodynamics:
Sum of electronic and zero-point Energies= -2641.607610

Sum of electronic and thermal Enthalpies= -2641.589958

Sum of electronic and thermal Free Energies= -2641.654028

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2641.777854

SCF energy, thermochemistry and PCM energy for **Cl⁻**.



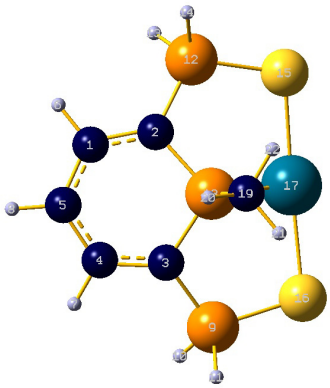
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.000000

HF=-460.1993284

thermodynamics:
Sum of electronic and zero-point Energies= -460.199328
Sum of electronic and thermal Enthalpies= -460.196968
Sum of electronic and thermal Free Energies= -460.214351

Total free energy in solution:
with all non electrostatic terms (a.u.) = -460.307396

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B1.**



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

1	6	0	1.222090	2.814983	-0.377150
2	6	0	1.384436	1.503130	0.074259
3	6	0	-1.385102	1.502542	0.074156
4	6	0	-1.223301	2.814486	-0.377138
5	6	0	-0.000735	3.478705	-0.506304
6	1	0	2.108931	3.350634	-0.716283
7	1	0	-2.110367	3.349796	-0.716223
8	1	0	-0.000942	4.499830	-0.870220
9	15	0	-2.838139	0.520711	-0.198537
10	1	0	-3.422439	0.950181	-1.409387
11	1	0	-3.864040	0.788030	0.729968
12	15	0	2.837774	0.521836	-0.198859
13	1	0	3.420986	0.950989	-1.410346
14	1	0	3.864163	0.790186	0.728798
15	16	0	2.387531	-1.459601	-0.117516
16	16	0	-2.386753	-1.460507	-0.118332
17	46	0	0.000420	-1.456258	-0.271173
18	15	0	-0.000136	0.552226	0.634237
19	6	0	-0.000490	0.288055	2.439757
20	1	0	-0.000797	1.261221	2.943262
21	1	0	-0.890152	-0.282202	2.724608
22	1	0	0.889021	-0.282080	2.725259

HF=-2181.3612993

	1			2			3		
	A			A			A		
Frequencies --	41.5416			49.5469			89.7645		
Red. masses --	7.4208			4.6042			21.2750		
Frc consts --	0.0075			0.0067			0.1010		
IR Inten --	0.2609			5.1989			2.7054		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.02	0.00	0.06	0.00	0.05	0.13	0.00	-0.01	-0.01
2 6	0.00	0.00	0.07	0.00	0.00	-0.03	0.00	-0.01	-0.01
3 6	0.00	0.00	-0.07	0.00	0.00	-0.03	0.00	-0.01	-0.01
4 6	0.02	0.00	-0.06	0.00	0.05	0.13	0.00	-0.01	-0.01
5 6	0.03	0.00	0.00	0.00	0.08	0.23	0.00	-0.01	-0.01
6 1	0.04	0.00	0.10	-0.01	0.08	0.16	0.00	-0.01	0.00
7 1	0.04	0.00	-0.10	0.01	0.08	0.16	0.00	-0.01	0.00
8 1	0.05	0.00	0.00	0.00	0.12	0.36	0.00	-0.01	0.00
9 15	0.03	-0.02	-0.15	0.04	-0.01	-0.18	0.01	-0.04	0.00
10 1	0.22	-0.22	-0.32	0.22	-0.11	-0.31	0.15	-0.26	-0.15
11 1	-0.11	0.14	-0.36	-0.10	0.06	-0.36	-0.09	0.13	-0.16
12 15	0.03	0.02	0.15	-0.04	-0.01	-0.18	-0.01	-0.04	0.00
13 1	0.22	0.22	0.32	-0.22	-0.11	-0.31	-0.16	-0.26	-0.15
14 1	-0.11	-0.14	0.36	0.10	0.06	-0.36	0.09	0.13	-0.16
15 16	0.01	0.01	-0.27	-0.01	-0.01	0.04	-0.01	-0.02	0.46
16 16	0.01	-0.01	0.27	0.01	-0.01	0.04	0.01	-0.02	0.46
17 46	-0.01	0.00	0.00	0.00	-0.02	0.04	0.00	0.08	-0.24
18 15	-0.03	0.00	0.00	0.00	0.00	-0.01	0.00	-0.02	-0.04
19 6	-0.09	0.00	0.00	0.00	0.06	0.00	0.00	-0.17	-0.07
20 1	-0.08	0.00	0.00	0.00	0.08	-0.04	0.00	-0.21	0.01
21 1	-0.10	0.01	-0.03	0.00	0.07	0.02	0.00	-0.19	-0.12
22 1	-0.10	-0.01	0.03	0.00	0.07	0.02	0.00	-0.19	-0.12

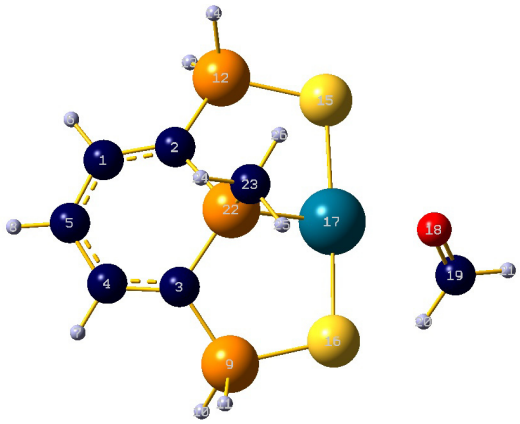
thermodynamics:
Sum of electronic and zero-point Energies= -2181.213620

Sum of electronic and thermal Enthalpies= -2181.198011

Sum of electronic and thermal Free Energies= -2181.256436

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2181.433710

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.240252	-0.789851	-0.734257
2	6	0	2.022765	-1.133355	-0.146810
3	6	0	1.627916	1.603959	-0.113846
4	6	0	2.894644	1.632181	-0.703778
5	6	0	3.707489	0.516476	-0.916839
6	1	0	3.855545	-1.590664	-1.145113
7	1	0	3.260518	2.584437	-1.088462
8	1	0	4.673773	0.660488	-1.386618
9	15	0	0.437577	2.897883	-0.209473
10	1	0	0.551945	3.544683	-1.460250
11	1	0	0.684646	3.965096	0.678349
12	15	0	1.239995	-2.709279	-0.273422
13	1	0	1.562566	-3.276894	-1.525842
14	1	0	1.773130	-3.668690	0.612148
15	16	0	-0.760118	-2.549703	0.088585
16	16	0	-1.430058	2.179618	0.198375
17	46	0	-1.160064	-0.191651	0.091056
18	8	0	-3.288182	-0.552313	-0.321023
19	6	0	-4.018345	0.015789	-1.115626
20	1	0	-3.665881	0.855777	-1.733426
21	1	0	-5.062767	-0.310445	-1.221846
22	15	0	0.977277	0.104388	0.592229
23	6	0	1.146719	0.103257	2.412381
24	1	0	2.198111	0.249521	2.682627
25	1	0	0.538476	0.908485	2.837214
26	1	0	0.789797	-0.851582	2.812134

HF=-2295.847417

	1			2			3		
	A			A			A		
Frequencies --	34.5818			39.9311			54.0076		
Red. masses --	4.7209			4.7602			4.3363		
Frc consts --	0.0033			0.0045			0.0075		
IR Inten --	5.3014			1.1535			12.1726		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.03	-0.01	0.08	0.07	0.01	0.12	-0.02	0.01	-0.05
2 6	0.02	0.00	0.06	0.00	0.00	-0.02	0.01	0.00	0.01
3 6	-0.01	0.00	-0.04	0.02	0.00	0.02	0.02	0.01	0.04
4 6	0.00	-0.01	-0.01	0.08	0.01	0.16	-0.01	0.01	-0.02
5 6	0.02	-0.01	0.05	0.10	0.01	0.23	-0.03	0.01	-0.09
6 1	0.05	-0.01	0.13	0.10	0.02	0.15	-0.03	0.01	-0.07
7 1	0.00	-0.02	-0.04	0.12	0.02	0.20	-0.03	0.02	-0.01
8 1	0.03	-0.01	0.07	0.16	0.02	0.35	-0.06	0.01	-0.14
9 15	-0.03	-0.03	-0.11	0.01	-0.02	-0.10	0.04	0.04	0.15
10 1	-0.15	-0.17	-0.20	0.01	-0.09	-0.13	0.18	0.23	0.26
11 1	0.02	0.08	-0.26	-0.02	0.04	-0.16	-0.03	-0.10	0.33
12 15	0.05	-0.02	0.10	-0.03	0.03	-0.17	0.03	-0.02	0.08
13 1	0.22	-0.11	0.19	-0.17	0.19	-0.27	0.06	-0.07	0.11
14 1	-0.05	0.06	0.25	0.04	-0.09	-0.35	0.04	0.04	0.13

15	16	0.00	-0.01	-0.19	0.01	0.01	0.06	0.03	-0.01	0.06
16	16	0.01	-0.01	0.13	0.00	0.00	-0.10	-0.01	0.00	-0.14
17	46	0.00	-0.01	-0.02	-0.01	0.00	-0.01	0.01	-0.01	-0.06
18	8	0.00	-0.02	-0.02	-0.02	-0.03	0.12	0.00	-0.05	-0.03
19	6	-0.09	0.17	0.20	-0.12	-0.02	0.21	-0.14	0.12	0.22
20	1	-0.18	0.38	0.43	-0.20	0.02	0.21	-0.28	0.32	0.42
21	1	-0.08	0.14	0.18	-0.12	-0.04	0.30	-0.13	0.07	0.26
22	15	-0.01	0.01	0.00	-0.01	-0.01	-0.01	0.00	-0.01	-0.01
23	6	-0.04	0.07	0.00	-0.01	-0.03	-0.01	-0.08	-0.04	0.00
24	1	-0.04	0.09	0.01	-0.01	-0.03	-0.01	-0.10	-0.04	0.05
25	1	-0.05	0.08	-0.04	-0.01	-0.03	0.00	-0.11	-0.05	-0.01
26	1	-0.04	0.08	0.03	-0.01	-0.03	-0.03	-0.10	-0.05	-0.03

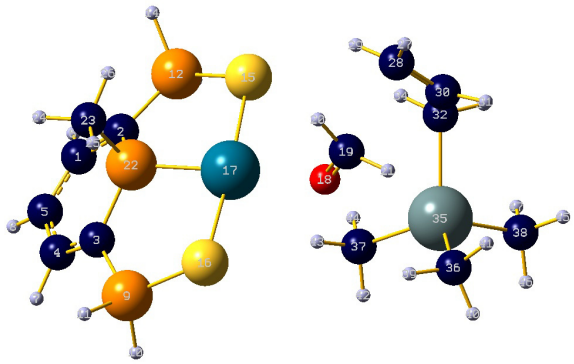
thermodynamics:
Sum of electronic and zero-point Energies= -2295.670246

Sum of electronic and thermal Enthalpies= -2295.650833

Sum of electronic and thermal Free Energies= -2295.718383

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2295.897213

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{B2B3}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.233240	1.378484	-1.931912
2	6	0	-3.316452	1.513487	-0.887203
3	6	0	-3.721022	-1.209284	-0.603546
4	6	0	-4.590396	-1.030732	-1.679477
5	6	0	-4.912844	0.201547	-2.258688
6	1	0	-4.393017	2.233655	-2.589040
7	1	0	-5.008368	-1.918292	-2.155234
8	1	0	-5.602488	0.216257	-3.095016
9	15	0	-3.002061	-2.741453	-0.112160
10	1	0	-2.788579	-3.539423	-1.258442
11	1	0	-3.883524	-3.557649	0.627699
12	15	0	-2.170108	2.835251	-0.702780
13	1	0	-1.802396	3.310870	-1.981327
14	1	0	-2.734474	3.996301	-0.133158
15	16	0	-0.588518	2.266207	0.457353
16	16	0	-1.328059	-2.425936	1.009450
17	46	0	-0.881806	-0.090516	0.745836
18	8	0	1.176758	-0.478948	1.262159
19	6	0	1.650006	-0.346086	2.414733
20	1	0	1.030201	0.001158	3.249776
21	1	0	2.564769	-0.887539	2.673186
22	15	0	-3.029694	0.185159	0.265145
23	6	0	-3.945451	0.480978	1.822372
24	1	0	-5.010982	0.611335	1.604837

25	1	0	-3.806098	-0.372042	2.494716
26	1	0	-3.555653	1.378981	2.313284
27	1	0	2.833567	1.631199	3.725621
28	6	0	2.644397	1.692507	2.656770
29	1	0	1.744999	2.221924	2.350737
30	6	0	3.645477	1.448754	1.763798
31	1	0	4.587738	1.065608	2.162193
32	6	0	3.568489	1.595333	0.317967
33	1	0	4.480258	2.065647	-0.070318
34	1	0	2.693841	2.164243	-0.008940
35	50	0	3.632907	-0.308216	-0.870200
36	6	0	4.002775	-2.040656	0.348260
37	6	0	1.870552	-0.461947	-2.089764
38	6	0	5.336634	0.021596	-2.144222
39	1	0	3.074025	-2.424078	0.778313
40	1	0	4.444647	-2.825617	-0.274179
41	1	0	4.710815	-1.821257	1.154054
42	1	0	1.993540	-1.270945	-2.817723
43	1	0	0.990317	-0.670639	-1.475037
44	1	0	1.708185	0.470814	-2.639387
45	1	0	6.250799	0.145164	-1.554123
46	1	0	5.481509	-0.830307	-2.816977
47	1	0	5.199689	0.918233	-2.757721

HF=-2536.1991598

		1			2			3		
		A			A			A		
Frequencies --		-49.4892			13.4354			17.5733		
Red. masses --		7.9860			5.7857			6.7228		
Frc consts --		0.0115			0.0006			0.0012		
IR Inten --		60.7530			0.2312			0.3288		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.02	0.03	0.04	-0.03	-0.05	0.17	-0.02	-0.12
2	6	0.01	-0.01	0.01	0.05	-0.02	-0.06	0.10	-0.01	-0.06
3	6	0.05	-0.01	0.03	-0.05	0.01	0.06	0.09	-0.01	-0.06
4	6	0.03	-0.03	0.04	-0.05	0.00	0.06	0.16	-0.02	-0.12
5	6	0.01	-0.03	0.04	-0.01	-0.02	0.01	0.19	-0.03	-0.16
6	1	-0.03	-0.03	0.03	0.07	-0.05	-0.09	0.21	-0.03	-0.13
7	1	0.03	-0.03	0.05	-0.09	-0.01	0.10	0.19	-0.03	-0.14
8	1	-0.01	-0.04	0.05	-0.01	-0.03	0.01	0.25	-0.04	-0.20
9	15	0.07	0.00	0.03	-0.11	0.00	0.13	0.06	-0.01	-0.01
10	1	0.03	-0.02	0.04	-0.19	-0.07	0.17	0.11	-0.02	0.01
11	1	0.10	0.01	0.07	-0.13	0.09	0.20	0.02	0.00	-0.05
12	15	-0.01	0.01	0.00	0.10	-0.05	-0.13	0.08	-0.01	0.00
13	1	-0.07	0.05	-0.01	0.15	-0.15	-0.15	0.14	0.00	0.02
14	1	-0.02	-0.01	0.04	0.14	0.01	-0.21	0.04	-0.01	-0.02
15	16	0.04	0.03	-0.07	0.05	-0.05	-0.06	0.02	0.00	0.09
16	16	0.11	0.02	-0.03	-0.06	-0.02	0.06	0.00	0.00	0.07
17	46	0.07	0.03	-0.02	0.00	-0.04	-0.01	0.02	0.00	0.06
18	8	0.07	0.12	-0.13	0.00	-0.08	-0.02	0.01	-0.01	0.09
19	6	0.03	0.15	-0.07	0.00	-0.14	-0.02	0.03	0.00	0.08
20	1	-0.12	-0.11	-0.07	0.00	-0.19	0.00	0.06	0.04	0.08
21	1	-0.08	-0.02	0.00	0.00	-0.15	-0.05	0.04	0.01	0.06
22	15	0.05	0.00	0.02	0.01	0.02	0.00	0.04	-0.01	-0.04
23	6	0.04	0.00	0.01	0.02	0.12	-0.01	-0.04	0.00	-0.08
24	1	0.04	-0.02	0.01	0.03	0.15	-0.01	-0.03	0.00	-0.13
25	1	0.05	0.00	0.02	0.00	0.15	0.03	-0.07	0.01	-0.07
26	1	0.03	0.00	0.01	0.06	0.13	-0.05	-0.06	0.01	-0.07
27	1	-0.28	-0.36	-0.04	-0.02	-0.19	0.10	0.12	0.03	0.03
28	6	-0.28	-0.38	-0.04	-0.01	-0.13	0.10	0.08	0.03	0.03
29	1	-0.22	-0.29	-0.04	-0.01	-0.12	0.13	0.07	0.04	0.07
30	6	-0.12	-0.08	0.00	-0.01	-0.09	0.09	0.03	0.00	-0.01
31	1	-0.11	-0.01	0.04	-0.01	-0.11	0.07	0.04	-0.02	-0.05
32	6	-0.03	0.03	0.06	0.00	0.00	0.10	-0.03	0.00	-0.01
33	1	0.05	-0.11	0.07	0.00	0.02	0.13	-0.04	-0.01	-0.04
34	1	0.02	0.06	-0.01	0.00	0.02	0.13	-0.03	0.01	0.03
35	50	-0.09	-0.03	0.03	0.00	0.07	-0.01	-0.10	0.01	-0.02
36	6	-0.08	-0.02	0.02	0.03	0.00	-0.10	-0.05	0.00	-0.06

37	6	-0.05	0.07	-0.03	0.00	0.11	-0.01	-0.16	0.02	0.06
38	6	-0.05	0.06	0.11	0.00	0.15	0.00	-0.18	0.01	-0.12
39	1	-0.08	0.01	0.05	0.03	-0.03	-0.11	-0.02	0.02	0.01
40	1	-0.13	-0.03	0.00	0.03	0.04	-0.15	-0.12	-0.01	-0.10
41	1	-0.04	-0.04	-0.01	0.03	-0.03	-0.09	0.02	-0.03	-0.12
42	1	-0.05	0.07	-0.03	0.02	0.15	-0.07	-0.21	0.01	0.06
43	1	-0.08	0.11	-0.06	0.01	0.05	-0.03	-0.14	0.05	0.09
44	1	0.02	0.08	-0.03	-0.02	0.14	0.04	-0.17	0.02	0.05
45	1	-0.07	0.03	0.14	0.00	0.12	0.00	-0.14	-0.01	-0.17
46	1	-0.02	0.08	0.08	0.00	0.19	-0.05	-0.23	0.02	-0.14
47	1	-0.04	0.08	0.14	-0.01	0.18	0.06	-0.20	0.02	-0.10

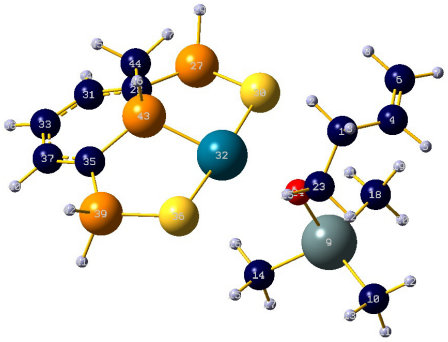
thermodynamics:
Sum of electronic and zero-point Energies= -2535.840124

Sum of electronic and thermal Enthalpies= -2535.807838

Sum of electronic and thermal Free Energies= -2535.906665

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2536.225922

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B3.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.345451	0.812647	2.728241
2	1	0	1.362341	1.302231	2.739693
3	1	0	2.572667	0.537313	3.769935
4	6	0	3.397857	1.755990	2.225247
5	1	0	4.419955	1.370266	2.229760
6	6	0	3.180756	3.007785	1.818896
7	1	0	3.994033	3.651698	1.494406
8	1	0	2.183064	3.442622	1.815156
9	50	0	2.781975	-0.630432	-1.082399
10	6	0	4.381505	-1.912126	-0.472193
11	1	0	4.889764	-2.290708	-1.365781
12	1	0	5.120887	-1.381465	0.134522
13	1	0	4.005824	-2.770914	0.092127
14	6	0	1.341336	-1.603363	-2.325418
15	1	0	0.981836	-2.516115	-1.841775
16	1	0	0.488430	-0.946060	-2.519767
17	1	0	1.795709	-1.871209	-3.285474
18	6	0	3.406354	1.284195	-1.788153
19	1	0	3.764733	1.887661	-0.950202
20	1	0	4.215806	1.168431	-2.516538
21	1	0	2.572409	1.806036	-2.264920
22	1	0	3.243994	-0.954710	1.862029
23	6	0	2.250428	-0.493392	1.941910
24	8	0	1.712427	-0.310586	0.626468
25	1	0	1.609396	-1.204073	2.479664

26	1	0	-1.839731	2.932345	-2.519864
27	15	0	-1.921455	2.696352	-1.128948
28	6	0	-3.111218	1.435327	-0.828835
29	1	0	-2.320420	3.967757	-0.664565
30	16	0	-0.133188	2.234403	-0.253294
31	6	0	-4.240619	1.184699	-1.610037
32	46	0	-0.418742	-0.008251	0.519497
33	6	0	-5.006261	0.015413	-1.565809
34	1	0	-4.520505	1.923915	-2.361008
35	6	0	-3.513675	-1.166584	0.022943
36	16	0	-0.844362	-2.245751	1.252239
37	6	0	-4.595720	-1.118232	-0.856345
38	1	0	-5.864069	-0.067548	-2.223533
39	15	0	-2.746091	-2.633703	0.620709
40	1	0	-5.132029	-2.044694	-1.063334
41	1	0	-2.831873	-3.638551	-0.369158
42	1	0	-3.447779	-3.241110	1.683703
43	15	0	-2.614864	0.310157	0.462487
44	6	0	-3.179392	0.925503	2.092014
45	1	0	-4.262499	1.086886	2.069734
46	1	0	-2.931376	0.192175	2.866654
47	1	0	-2.670465	1.865933	2.328260

HF=-2536.2616829

		1			2			3		
		A			A			A		
Frequencies --		11.0883			20.2746			23.7940		
Red. masses --		4.1349			2.7622			3.7684		
Frc consts --		0.0003			0.0007			0.0013		
IR Inten --		0.0706			0.1238			0.2233		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.05	-0.12	0.05	-0.03	0.04	-0.01	0.09	-0.04	0.01
2	1	-0.08	-0.17	0.08	-0.04	0.03	-0.03	0.12	0.03	0.01
3	1	-0.03	-0.16	0.03	-0.05	0.05	-0.01	0.07	-0.05	0.01
4	6	-0.10	-0.03	0.10	-0.03	0.05	0.00	0.16	-0.11	0.01
5	1	-0.08	0.03	0.07	-0.03	0.06	0.02	0.13	-0.18	0.04
6	6	-0.18	-0.02	0.17	-0.04	0.05	-0.01	0.24	-0.11	-0.02
7	1	-0.21	0.04	0.20	-0.04	0.05	0.00	0.29	-0.17	-0.02
8	1	-0.20	-0.08	0.19	-0.04	0.04	-0.03	0.27	-0.04	-0.04
9	50	0.00	0.03	-0.03	0.02	-0.01	0.01	-0.02	0.05	0.00
10	6	-0.02	-0.02	-0.08	-0.11	-0.17	0.02	-0.05	-0.01	-0.04
11	1	-0.03	0.00	-0.10	-0.14	-0.23	0.03	-0.06	0.01	-0.05
12	1	-0.01	-0.06	-0.07	-0.06	-0.23	0.03	-0.04	-0.05	-0.02
13	1	-0.03	-0.03	-0.11	-0.20	-0.12	0.03	-0.07	-0.02	-0.07
14	6	-0.01	0.10	-0.07	-0.03	0.15	-0.06	-0.05	0.12	-0.02
15	1	-0.05	0.11	-0.09	-0.08	0.14	-0.12	-0.08	0.12	-0.04
16	1	0.01	0.13	-0.07	0.01	0.21	-0.03	-0.03	0.15	-0.01
17	1	-0.01	0.10	-0.07	-0.04	0.18	-0.08	-0.06	0.12	-0.03
18	6	0.04	0.06	0.07	0.20	-0.05	0.07	0.03	0.04	0.03
19	1	-0.21	0.10	0.15	0.52	-0.20	0.04	0.33	-0.08	-0.01
20	1	0.23	0.10	0.28	0.00	-0.12	-0.14	-0.18	0.00	-0.19
21	1	0.12	-0.01	-0.14	0.18	0.15	0.33	-0.03	0.18	0.30
22	1	0.04	-0.02	-0.05	0.00	0.05	0.00	-0.04	-0.10	0.00
23	6	0.02	-0.08	-0.03	-0.01	0.04	-0.01	-0.01	-0.03	0.01
24	8	0.01	-0.03	-0.01	0.00	0.02	-0.02	-0.01	0.01	0.02
25	1	0.06	-0.14	-0.06	0.00	0.03	-0.01	-0.05	0.01	0.02
26	1	0.06	-0.13	-0.11	-0.06	0.01	0.01	0.05	-0.07	-0.05
27	15	0.05	-0.06	-0.10	-0.04	0.00	0.01	0.00	-0.03	-0.05
28	6	0.03	-0.02	-0.04	-0.03	0.00	0.02	0.01	-0.04	-0.06
29	1	0.07	-0.02	-0.17	-0.04	0.00	0.02	-0.02	-0.03	-0.10
30	16	0.04	-0.04	-0.06	-0.02	0.01	-0.01	-0.02	0.00	0.02
31	6	0.01	-0.03	-0.01	-0.04	-0.01	0.04	0.04	-0.07	-0.09
32	46	0.01	-0.01	0.00	0.00	0.01	-0.02	-0.01	0.00	0.02
33	6	-0.01	-0.01	0.04	-0.03	-0.01	0.04	0.04	-0.07	-0.08
34	1	0.02	-0.05	-0.04	-0.05	0.00	0.04	0.05	-0.09	-0.11
35	6	-0.01	0.02	0.06	0.00	-0.01	0.01	0.00	-0.02	0.00
36	16	-0.01	0.01	0.05	0.02	0.00	-0.03	-0.01	0.00	0.03
37	6	-0.02	0.01	0.07	-0.01	-0.01	0.03	0.03	-0.05	-0.03

38	1	-0.02	-0.02	0.05	-0.04	-0.01	0.05	0.07	-0.10	-0.11
39	15	-0.03	0.02	0.10	0.01	-0.01	0.00	-0.02	0.00	0.07
40	1	-0.04	0.01	0.11	-0.01	-0.01	0.03	0.04	-0.06	-0.02
41	1	-0.06	-0.01	0.13	0.01	-0.01	0.00	-0.04	-0.04	0.11
42	1	-0.02	0.07	0.13	0.03	-0.01	0.01	-0.02	0.06	0.10
43	15	0.02	0.02	0.00	0.00	-0.01	0.01	-0.02	-0.01	-0.02
44	6	0.03	0.09	-0.02	0.01	-0.02	0.02	-0.05	0.03	-0.04
45	1	0.04	0.10	-0.02	0.01	-0.03	0.03	-0.05	0.03	-0.07
46	1	0.02	0.11	0.01	0.03	-0.02	0.01	-0.06	0.06	-0.02
47	1	0.05	0.08	-0.05	0.01	-0.02	0.02	-0.05	0.04	-0.06

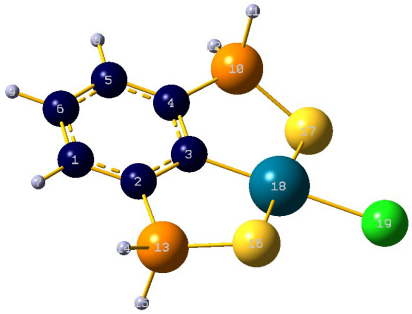
thermodynamics:
Sum of electronic and zero-point Energies= -2535.899717

Sum of electronic and thermal Enthalpies= -2535.867115

Sum of electronic and thermal Free Energies= -2535.968056
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2536.287457

S~C~*S* complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B0.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.227393	-1.198228	0.110176
2	6	0	1.829292	-1.184511	0.106355
3	6	0	1.063050	-0.000133	0.000591
4	6	0	1.829682	1.183903	-0.105195
5	6	0	3.227850	1.196938	-0.110980
6	6	0	3.931311	-0.000794	-0.000932
7	1	0	3.775252	-2.134393	0.197793
8	1	0	3.776004	2.132901	-0.198967
9	1	0	5.017086	-0.001102	-0.001727
10	15	0	0.827078	2.663527	-0.264051
11	1	0	0.883668	3.071972	-1.616921
12	1	0	1.514841	3.729409	0.359845
13	15	0	0.825844	-2.663548	0.264978
14	1	0	1.513825	-3.729851	-0.357926
15	1	0	0.880628	-3.071729	1.617990
16	16	0	-1.025283	-2.327857	-0.434311
17	16	0	-1.024574	2.328352	0.433757
18	46	0	-0.951239	0.000137	-0.000022
19	17	0	-3.308935	0.000342	-0.000248

HF=-2298.6416932

	1	2	3
	A	A	A
Frequencies --	44.7490	52.9969	67.8097

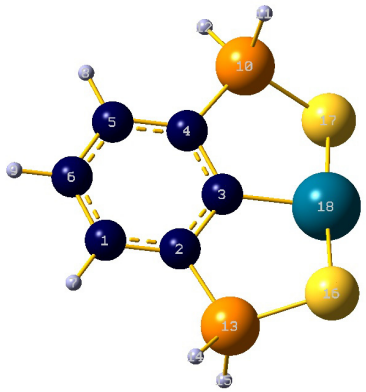
Red. masses --		6.3466			8.9845			4.9832		
Frc consts --		0.0075			0.0149			0.0135		
IR Inten --		0.9780			2.0454			4.2202		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	-0.09	-0.01	0.01	0.20	-0.02	-0.02	-0.05
2	6	0.00	-0.01	-0.08	-0.01	0.00	0.01	-0.01	0.01	0.01
3	6	-0.01	0.00	0.00	0.00	-0.01	-0.06	0.00	0.02	0.00
4	6	0.00	0.01	0.08	0.01	0.00	0.01	0.01	0.01	0.01
5	6	0.00	0.00	0.09	0.01	0.01	0.20	0.02	-0.02	-0.05
6	6	0.01	0.00	0.00	0.00	0.02	0.32	0.00	-0.03	-0.11
7	1	0.00	-0.01	-0.16	-0.01	0.02	0.27	-0.03	-0.03	-0.06
8	1	0.00	0.01	0.15	0.01	0.02	0.27	0.03	-0.03	-0.06
9	1	0.01	0.00	0.00	0.00	0.03	0.48	0.00	-0.05	-0.17
10	15	0.07	0.06	0.14	0.00	-0.03	-0.15	0.07	0.06	0.14
11	1	0.32	0.26	0.21	0.01	-0.16	-0.19	0.26	0.32	0.23
12	1	0.00	-0.06	0.41	-0.01	0.04	-0.25	0.02	-0.07	0.43
13	15	0.07	-0.06	-0.14	0.00	-0.03	-0.15	-0.07	0.06	0.14
14	1	0.00	0.06	-0.40	0.01	0.04	-0.25	-0.02	-0.07	0.43
15	1	0.32	-0.26	-0.21	0.00	-0.17	-0.19	-0.26	0.32	0.23
16	16	-0.07	-0.03	0.22	0.00	0.02	-0.13	0.04	-0.01	-0.15
17	16	-0.07	0.03	-0.22	0.00	0.02	-0.13	-0.04	-0.01	-0.15
18	46	-0.01	0.00	0.00	0.00	0.00	-0.02	0.00	-0.02	-0.02
19	17	-0.01	0.00	0.00	0.00	-0.01	0.32	0.00	-0.04	0.12

thermodynamics:
Sum of electronic and zero-point Energies= -2298.526999

Sum of electronic and thermal Enthalpies= -2298.512427

Sum of electronic and thermal Free Energies= -2298.569372
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2298.670559

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B1.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002770	-0.013319	-0.009130
2	6	0	-0.009354	-0.013496	1.390821
3	6	0	1.190725	0.002560	2.128341
4	6	0	2.398981	0.019941	1.404351
5	6	0	2.408037	0.022407	0.004413
6	6	0	1.206544	0.005211	-0.699982
7	1	0	-0.937619	-0.016308	-0.564292
8	1	0	3.349040	0.026435	-0.540250
9	1	0	1.212635	0.006258	-1.785196
10	15	0	3.868399	-0.021454	2.432496
11	1	0	4.377561	1.286419	2.560932
12	1	0	4.886147	-0.694977	1.732000

13	15	0	-1.490177	0.026077	2.402577
14	1	0	-2.500123	0.700552	1.691813
15	1	0	-2.000479	-1.282077	2.523309
16	16	0	-1.004691	0.910780	4.149884
17	16	0	3.363476	-0.908873	4.172882
18	46	0	1.179767	0.001031	4.086484

HF=-1838.2410689

	1			2			3		
	A			A			A		
Frequencies --	67.7575			76.3756			103.1826		
Red. masses --	7.0695			4.8515			17.6770		
Frc consts --	0.0191			0.0167			0.1109		
IR Inten --	2.3307			5.7171			0.5833		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.00	-0.11	0.01	0.00	0.11	0.01	0.04	-0.09	-0.01
2 6	0.00	-0.11	0.01	0.02	-0.01	0.01	0.02	0.08	-0.01
3 6	0.00	0.00	0.00	0.02	-0.02	0.00	0.01	0.15	0.00
4 6	0.00	0.10	0.01	0.02	-0.01	-0.01	0.02	0.08	0.01
5 6	0.00	0.11	0.01	0.00	0.11	-0.01	0.04	-0.09	0.01
6 6	0.00	0.00	0.02	-0.01	0.20	0.00	0.05	-0.18	0.00
7 1	0.00	-0.20	0.01	-0.01	0.14	0.02	0.05	-0.16	-0.02
8 1	0.00	0.20	0.01	-0.01	0.14	-0.02	0.05	-0.16	0.02
9 1	0.00	0.00	0.02	-0.02	0.32	0.00	0.06	-0.32	0.00
10 15	-0.05	0.14	0.09	0.04	-0.19	-0.05	-0.03	0.01	0.07
11 1	-0.22	0.18	0.34	0.28	-0.27	-0.14	-0.12	0.02	0.35
12 1	0.08	0.38	0.05	-0.10	-0.41	-0.03	0.05	0.20	0.01
13 15	0.05	-0.14	0.09	0.04	-0.19	0.05	-0.03	0.01	-0.07
14 1	-0.08	-0.37	0.05	-0.10	-0.41	0.03	0.05	0.19	0.00
15 1	0.21	-0.18	0.34	0.28	-0.27	0.15	-0.11	0.02	-0.35
16 16	0.08	0.21	-0.09	-0.04	0.01	-0.03	-0.15	-0.34	0.15
17 16	-0.08	-0.21	-0.09	-0.05	0.00	0.03	-0.15	-0.35	-0.15
18 46	0.00	0.00	-0.01	0.00	0.07	0.00	0.08	0.21	0.00

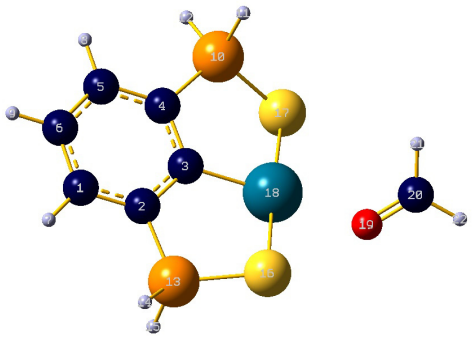
thermodynamics:
Sum of electronic and zero-point Energies= -1838.126632

Sum of electronic and thermal Enthalpies= -1838.114058

Sum of electronic and thermal Free Energies= -1838.165695

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1838.321593

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.021099	0.056767	-0.024225
2	6	0	-0.064593	-0.064331	1.367298
3	6	0	1.073684	-0.070640	2.203413
4	6	0	2.313374	0.057745	1.538388

5	6	0	2.416501	0.185247	0.148295
6	6	0	1.265909	0.182942	-0.635230
7	1	0	-0.877706	0.059603	-0.636313
8	1	0	3.388905	0.279314	-0.329344
9	1	0	1.338748	0.278657	-1.713790
10	15	0	3.734816	0.025216	2.626399
11	1	0	4.194911	1.342802	2.828802
12	1	0	4.816360	-0.576135	1.954956
13	15	0	-1.617769	-0.199635	2.250211
14	1	0	-2.604059	0.520434	1.549081
15	1	0	-2.082687	-1.527627	2.157120
16	16	0	-1.329479	0.450839	4.133765
17	16	0	3.209854	-0.940339	4.316813
18	46	0	0.942896	-0.247233	4.174997
19	8	0	0.742093	-0.476777	6.322152
20	6	0	1.409071	0.017956	7.216533
21	1	0	2.272956	0.666907	7.010842
22	1	0	1.146302	-0.190704	8.262991

HF=-1952.7319479

		1			2			3		
		A			A			A		
Frequencies --		43.1231			53.4126			61.8329		
Red. masses --		3.3208			4.8420			6.1679		
Frc consts --		0.0036			0.0081			0.0139		
IR Inten --		10.7572			5.5375			2.4634		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.10	-0.01	0.03	0.09	-0.01	-0.01	-0.05	0.01
2	6	0.00	-0.05	-0.01	0.00	0.00	-0.02	0.00	-0.08	0.01
3	6	0.00	0.01	0.00	-0.01	-0.02	0.00	0.01	-0.01	0.00
4	6	0.00	0.01	0.01	0.00	0.01	0.03	0.00	0.09	0.01
5	6	0.01	-0.04	0.00	0.02	0.10	0.04	-0.01	0.13	0.02
6	6	0.01	-0.10	-0.01	0.03	0.15	0.02	-0.02	0.07	0.02
7	1	0.01	-0.15	-0.02	0.03	0.12	-0.02	-0.01	-0.10	0.01
8	1	0.01	-0.04	0.00	0.03	0.14	0.06	-0.02	0.22	0.02
9	1	0.02	-0.15	-0.01	0.05	0.22	0.03	-0.02	0.11	0.02
10	15	-0.02	0.07	0.03	-0.01	-0.05	0.04	-0.04	0.07	0.06
11	1	-0.10	0.09	0.08	0.02	-0.07	0.09	-0.15	0.09	0.25
12	1	0.03	0.15	0.04	-0.02	-0.05	0.03	0.04	0.25	0.03
13	15	0.00	-0.02	0.00	0.00	-0.07	-0.04	0.05	-0.16	0.08
14	1	-0.01	-0.06	-0.03	-0.02	-0.09	-0.04	-0.08	-0.42	0.00
15	1	0.02	-0.03	0.07	0.05	-0.08	-0.08	0.24	-0.24	0.34
16	16	0.00	0.08	-0.03	-0.05	-0.10	-0.02	0.07	0.22	-0.05
17	16	-0.02	0.00	-0.01	-0.05	-0.10	0.00	-0.04	-0.19	-0.09
18	46	-0.01	0.03	0.00	-0.02	0.00	0.00	0.00	-0.01	-0.01
19	8	-0.05	0.03	0.00	0.03	0.26	0.05	0.00	-0.02	-0.01
20	6	0.17	-0.31	0.03	0.29	0.11	-0.06	-0.10	0.13	-0.02
21	1	0.44	-0.66	0.06	0.54	-0.27	-0.21	-0.23	0.29	-0.02
22	1	0.09	-0.28	0.01	0.29	0.35	-0.02	-0.07	0.10	-0.01

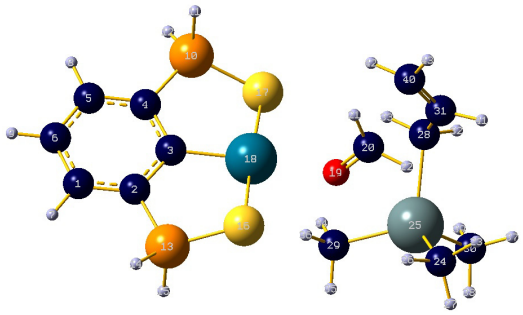
thermodynamics:
Sum of electronic and zero-point Energies= -1952.587641

Sum of electronic and thermal Enthalpies= -1952.571405

Sum of electronic and thermal Free Energies= -1952.631760

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1952.789268

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{B2B3}.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.170928	-1.035437	-0.932946
2	6	0	-3.862957	-1.100122	-0.439609
3	6	0	-3.061505	0.045593	-0.228216
4	6	0	-3.687261	1.272347	-0.548544
5	6	0	-4.995440	1.358470	-1.038623
6	6	0	-5.740145	0.198908	-1.233809
7	1	0	-5.753428	-1.942076	-1.080362
8	1	0	-5.437584	2.323830	-1.274144
9	1	0	-6.754524	0.256430	-1.615302
10	15	0	-2.660694	2.713248	-0.275916
11	1	0	-3.072396	3.350775	0.913465
12	1	0	-2.962592	3.683935	-1.251214
13	15	0	-3.066449	-2.647273	-0.013952
14	1	0	-4.039191	-3.531726	0.492860
15	1	0	-2.668012	-3.295645	-1.201996
16	16	0	-1.561667	-2.272660	1.266901
17	16	0	-0.730739	2.140602	-0.282017
18	46	0	-1.197863	-0.062362	0.473565
19	8	0	0.794179	-0.287732	1.187956
20	6	0	1.186172	0.021810	2.340087
21	1	0	0.500206	0.456285	3.076200
22	1	0	2.082380	-0.466612	2.731703
23	1	0	4.422554	-1.553395	1.635054
24	6	0	3.814844	-1.881103	0.785400
25	50	0	3.636368	-0.342544	-0.705231
26	1	0	2.829577	-2.191775	1.142651
27	1	0	4.309666	-2.751274	0.341680
28	6	0	3.390459	1.697097	0.204945
29	6	0	2.027955	-0.686103	-2.085181
30	6	0	5.495201	-0.148863	-1.769047
31	6	0	3.261277	1.736934	1.652908
32	1	0	4.345963	2.135931	-0.107813
33	1	0	2.570475	2.200732	-0.314336
34	1	0	1.920661	0.159555	-2.771689
35	1	0	2.232775	-1.583827	-2.678064
36	1	0	1.087094	-0.826978	-1.546142
37	1	0	6.320038	0.064007	-1.081144
38	1	0	5.729399	-1.076309	-2.302001
39	1	0	5.440868	0.660775	-2.504016
40	6	0	2.140433	2.059474	2.362960
41	1	0	4.144634	1.440003	2.222964
42	1	0	1.285274	2.514611	1.869158
43	1	0	2.193033	2.159714	3.444361

HF=-2193.0855409

	1 A	2 A	3 A
Frequencies --	-69.9095	12.7818	18.4117
Red. masses --	7.0537	6.7819	7.1796
Frc consts --	0.0203	0.0007	0.0014
IR Inten --	121.3724	0.1851	0.6546

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.03	-0.02	0.04	-0.09	0.07	0.12	-0.09	0.00	0.12
2	6	0.03	0.00	0.03	-0.08	0.03	0.08	-0.07	0.00	0.05
3	6	0.03	0.00	0.02	-0.02	0.00	0.02	-0.07	0.01	0.03
4	6	0.01	-0.01	0.01	0.02	0.02	-0.02	-0.10	0.01	0.09
5	6	0.01	-0.02	0.02	0.01	0.05	0.01	-0.13	0.01	0.17
6	6	0.02	-0.02	0.03	-0.04	0.08	0.08	-0.13	0.00	0.19
7	1	0.03	-0.02	0.04	-0.13	0.09	0.17	-0.09	0.00	0.14
8	1	0.00	-0.02	0.01	0.05	0.06	-0.01	-0.15	0.01	0.22
9	1	0.02	-0.03	0.03	-0.05	0.11	0.10	-0.15	0.00	0.25
10	15	0.00	0.01	0.00	0.09	-0.01	-0.10	-0.10	0.01	0.06
11	1	0.01	0.00	0.01	0.14	0.05	-0.12	-0.05	-0.01	0.09
12	1	-0.03	0.01	0.01	0.11	-0.04	-0.14	-0.15	0.03	0.10
13	15	0.04	0.01	0.04	-0.13	0.01	0.12	-0.03	0.00	-0.03
14	1	0.06	0.02	0.09	-0.15	0.07	0.18	0.01	-0.02	0.00
15	1	-0.01	-0.02	0.03	-0.19	-0.05	0.14	-0.08	0.04	-0.07
16	16	0.10	0.02	-0.03	-0.08	0.00	0.06	0.04	-0.01	-0.10
17	16	0.01	0.04	-0.02	0.07	-0.09	-0.12	-0.09	0.03	-0.04
18	46	0.06	0.03	-0.01	-0.01	-0.05	-0.03	-0.03	0.02	-0.05
19	8	0.07	0.12	-0.11	0.00	-0.08	-0.07	-0.01	0.04	-0.10
20	6	0.03	0.21	-0.06	0.00	-0.15	-0.05	-0.02	0.04	-0.09
21	1	-0.14	-0.06	-0.06	-0.01	-0.23	-0.01	-0.03	0.03	-0.10
22	1	-0.13	0.01	0.06	0.02	-0.15	-0.09	-0.02	0.04	-0.09
23	1	0.05	-0.03	-0.03	0.02	0.01	-0.02	-0.05	0.02	0.11
24	6	-0.03	-0.01	0.03	0.07	0.01	-0.06	0.01	0.00	0.07
25	50	-0.05	-0.04	0.02	0.04	0.06	0.00	0.10	-0.03	0.03
26	1	-0.03	0.07	0.10	0.07	-0.06	-0.11	-0.01	-0.01	0.01
27	1	-0.12	-0.04	0.00	0.14	0.05	-0.07	0.05	0.00	0.12
28	6	-0.01	0.04	0.04	-0.05	0.02	0.07	0.05	-0.01	-0.04
29	6	-0.04	0.06	-0.01	0.08	0.05	-0.04	0.17	-0.05	-0.04
30	6	-0.04	0.07	0.07	0.05	0.16	0.04	0.17	-0.07	0.14
31	6	-0.12	-0.08	-0.02	-0.07	-0.05	0.07	0.00	0.03	-0.04
32	1	0.08	-0.12	0.10	-0.06	0.06	0.10	0.06	-0.01	-0.01
33	1	0.06	0.05	-0.05	-0.06	0.01	0.08	0.07	-0.03	-0.08
34	1	-0.01	0.08	0.02	0.04	0.08	0.00	0.22	-0.07	-0.08
35	1	-0.03	0.08	-0.04	0.14	0.09	-0.09	0.18	-0.07	0.00
36	1	-0.03	0.05	-0.02	0.08	-0.04	-0.07	0.14	-0.01	-0.09
37	1	-0.05	0.06	0.09	0.03	0.17	0.07	0.12	-0.05	0.18
38	1	-0.01	0.10	0.03	0.10	0.19	0.01	0.20	-0.09	0.18
39	1	-0.05	0.10	0.10	0.04	0.19	0.07	0.22	-0.09	0.11
40	6	-0.30	-0.42	-0.06	-0.09	-0.13	0.07	-0.04	0.03	-0.09
41	1	-0.12	0.01	0.02	-0.06	-0.04	0.07	-0.02	0.05	0.00
42	1	-0.22	-0.31	-0.08	-0.10	-0.14	0.08	-0.02	0.02	-0.13
43	1	-0.28	-0.33	-0.07	-0.11	-0.17	0.08	-0.07	0.06	-0.09

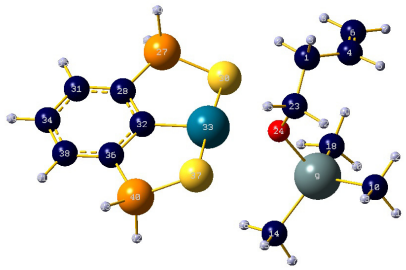
thermodynamics:
Sum of electronic and zero-point Energies= -2192.759544

Sum of electronic and thermal Enthalpies= -2192.730326

Sum of electronic and thermal Free Energies= -2192.822507

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2193.119564

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B3.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.019301	0.035547	0.025423
2	1	0	-0.032764	0.029164	1.121939
3	1	0	1.037747	0.068613	-0.281564
4	6	0	-0.718587	1.253360	-0.503149
5	1	0	-0.699700	1.377865	-1.588222
6	6	0	-1.306471	2.189374	0.244272
7	1	0	-1.764652	3.069693	-0.199214
8	1	0	-1.329978	2.119762	1.330099
9	50	0	-3.629069	-1.363993	-0.935042
10	6	0	-3.062829	-1.000480	-2.963137
11	1	0	-3.971419	-0.931429	-3.571313
12	1	0	-2.515734	-0.059527	-3.065070
13	1	0	-2.452676	-1.816762	-3.361108
14	6	0	-4.611509	-3.240345	-0.644438
15	1	0	-4.004941	-4.057773	-1.043471
16	1	0	-4.793754	-3.416454	0.420215
17	1	0	-5.577639	-3.233812	-1.160857
18	6	0	-4.629906	0.251158	0.035750
19	1	0	-3.958611	1.109482	0.117159
20	1	0	-5.508872	0.542820	-0.549177
21	1	0	-4.961901	-0.042895	1.035568
22	1	0	-0.666358	-1.256215	-1.588020
23	6	0	-0.579794	-1.287204	-0.493709
24	8	0	-1.861472	-1.617367	0.064218
25	1	0	0.111117	-2.102606	-0.248190
26	1	0	-2.571641	-0.859088	5.915829
27	15	0	-1.799936	-1.341959	4.840189
28	6	0	-1.807258	-3.131698	4.881485
29	1	0	-0.508081	-0.887632	5.179925
30	16	0	-2.438500	-0.719873	3.035590
31	6	0	-1.797089	-3.850507	6.082524
32	6	0	-1.817259	-3.750386	3.609300
33	46	0	-1.830477	-2.713840	1.902271
34	6	0	-1.799853	-5.242006	6.059726
35	1	0	-1.790371	-3.332360	7.038892
36	6	0	-1.817457	-5.164794	3.644215
37	16	0	-1.189690	-4.634396	0.657366
38	6	0	-1.810774	-5.901547	4.834226
39	1	0	-1.793086	-5.806150	6.986808
40	15	0	-1.832159	-5.950428	2.034990
41	1	0	-1.809746	-6.989062	4.813288
42	1	0	-3.126737	-6.456488	1.791289
43	1	0	-1.063678	-7.129908	2.096866

HF=-2193.1466588

	1			2			3		
	A			A			A		
Frequencies --	20.3084			24.2880			27.2836		
Red. masses --	4.2167			4.9768			4.0548		
Frc consts --	0.0010			0.0017			0.0018		
IR Inten --	0.0227			0.2779			0.6856		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.04	-0.09	0.05	-0.03	0.03	0.09	0.02	-0.08	0.00

2	1	0.11	-0.18	0.05	-0.02	-0.03	0.09	0.00	-0.08	-0.01
3	1	0.03	-0.10	-0.01	-0.04	0.07	0.08	0.03	-0.10	0.02
4	6	0.05	-0.02	0.19	-0.07	0.04	0.16	0.05	-0.07	-0.02
5	1	-0.04	0.05	0.20	-0.08	0.10	0.17	0.11	-0.06	-0.02
6	6	0.16	-0.05	0.31	-0.09	-0.02	0.21	0.01	-0.08	-0.04
7	1	0.17	0.01	0.41	-0.12	-0.01	0.27	0.04	-0.07	-0.06
8	1	0.25	-0.13	0.31	-0.08	-0.08	0.21	-0.04	-0.09	-0.04
9	50	-0.03	0.00	-0.02	0.01	-0.04	-0.05	0.00	0.04	-0.01
10	6	-0.02	-0.08	-0.03	0.06	0.07	-0.02	-0.01	0.26	0.03
11	1	-0.01	-0.08	-0.04	0.07	0.07	-0.04	-0.02	0.33	0.05
12	1	0.01	-0.10	-0.06	0.03	0.10	0.04	-0.01	0.27	0.13
13	1	-0.04	-0.11	0.00	0.09	0.11	-0.04	-0.02	0.30	-0.07
14	6	-0.08	0.04	0.06	0.06	-0.08	-0.16	0.02	0.00	-0.21
15	1	-0.11	0.01	0.06	0.11	-0.05	-0.15	0.06	0.04	-0.23
16	1	-0.05	0.08	0.07	0.01	-0.12	-0.18	-0.03	-0.09	-0.23
17	1	-0.09	0.06	0.09	0.09	-0.10	-0.21	0.05	0.02	-0.26
18	6	0.04	0.08	-0.08	-0.07	-0.11	0.00	-0.02	-0.06	0.15
19	1	0.09	0.04	-0.07	-0.10	-0.08	0.03	-0.03	-0.06	0.22
20	1	0.08	0.12	-0.12	-0.07	-0.13	0.00	-0.03	-0.03	0.19
21	1	-0.01	0.11	-0.09	-0.06	-0.15	-0.01	0.00	-0.15	0.13
22	1	-0.06	0.06	-0.03	0.01	0.08	0.03	0.01	-0.07	-0.01
23	6	-0.03	-0.03	-0.03	-0.01	0.04	0.03	0.00	-0.07	-0.01
24	8	-0.02	-0.02	-0.03	-0.01	0.00	0.00	-0.01	-0.05	-0.02
25	1	-0.05	-0.08	-0.12	0.00	0.04	0.00	-0.01	-0.08	-0.01
26	1	-0.10	0.01	-0.04	0.26	0.07	0.04	-0.08	0.02	-0.04
27	15	-0.06	0.03	-0.02	0.15	0.02	-0.02	-0.05	0.02	-0.02
28	6	0.00	0.03	-0.01	0.09	0.02	0.00	0.00	0.02	0.00
29	1	-0.08	0.07	0.01	0.20	-0.02	-0.14	-0.07	0.06	-0.01
30	16	-0.03	0.00	-0.04	0.02	0.01	0.02	-0.05	-0.02	-0.03
31	6	0.03	0.04	-0.01	0.11	0.03	0.01	0.03	0.05	0.02
32	6	0.01	0.01	-0.01	0.01	0.02	0.01	0.01	0.00	0.01
33	46	-0.01	0.00	-0.02	-0.01	0.01	0.00	-0.02	-0.03	0.00
34	6	0.07	0.04	0.01	0.04	0.03	0.01	0.08	0.05	0.04
35	1	0.01	0.05	-0.01	0.17	0.03	0.00	0.03	0.06	0.01
36	6	0.06	0.01	0.01	-0.05	0.02	0.01	0.05	0.00	0.04
37	16	-0.01	0.00	-0.01	-0.05	-0.01	0.01	-0.02	-0.04	0.02
38	6	0.09	0.03	0.02	-0.04	0.02	0.01	0.09	0.02	0.05
39	1	0.10	0.05	0.02	0.06	0.03	0.01	0.11	0.06	0.05
40	15	0.07	-0.01	0.02	-0.14	0.03	0.01	0.06	-0.03	0.06
41	1	0.13	0.03	0.03	-0.09	0.02	0.02	0.12	0.02	0.07
42	1	0.09	-0.07	0.05	-0.18	0.13	0.02	0.07	-0.09	0.09
43	1	0.12	0.02	0.03	-0.23	-0.03	-0.01	0.11	0.00	0.07

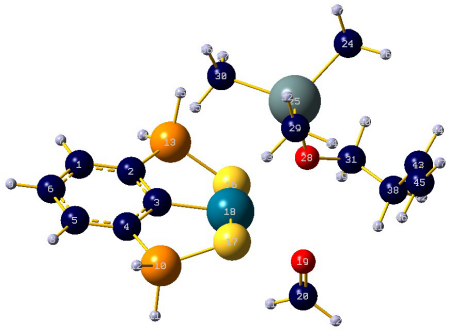
```
thermodynamics:
Sum of electronic and zero-point Energies=          -2192.817342

Sum of electronic and thermal Enthalpies=           -2192.788091

Sum of electronic and thermal Free Energies=        -2192.880221

 Total free energy in solution:
  with all non electrostatic terms            (a.u.) =   -2193.180723
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{B3B2}.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.337136	-1.642512	-0.785777
2	6	0	3.184623	-0.865043	-0.941902
3	6	0	2.548972	-0.210581	0.139556
4	6	0	3.169655	-0.391193	1.398556
5	6	0	4.324454	-1.163238	1.568875
6	6	0	4.909661	-1.793524	0.474357
7	1	0	4.796355	-2.127754	-1.643912
8	1	0	4.769963	-1.279469	2.554195
9	1	0	5.804641	-2.393939	0.601485
10	15	0	2.344887	0.451886	2.743282
11	1	0	3.057618	1.632149	3.044511
12	1	0	2.510038	-0.301785	3.922408
13	15	0	2.390419	-0.588114	-2.520478
14	1	0	3.367381	-0.629250	-3.534918
15	1	0	1.583135	-1.702154	-2.828813
16	16	0	1.389287	1.151846	-2.419385
17	16	0	0.424943	0.742438	2.214417
18	46	0	0.920732	0.886059	-0.098170
19	8	0	-0.198238	3.031798	-0.193677
20	6	0	0.365043	4.078149	-0.446749
21	1	0	1.412288	4.110594	-0.792693
22	1	0	-0.164708	5.038895	-0.339074
23	1	0	-3.629579	-1.810974	-2.334453
24	6	0	-3.875198	-2.003093	-1.285403
25	50	0	-2.231329	-1.518433	0.000480
26	1	0	-4.773864	-1.440300	-1.022424
27	1	0	-4.096488	-3.071042	-1.181065
28	8	0	-1.616097	0.336818	-0.440021
29	6	0	-2.664259	-1.667732	2.088887
30	6	0	-0.533420	-2.729939	-0.520685
31	6	0	-2.397545	1.190153	-1.266624
32	1	0	-2.970371	-2.692924	2.324364
33	1	0	-1.782423	-1.421610	2.686579
34	1	0	-3.477207	-0.988190	2.354953
35	1	0	0.383421	-2.320269	-0.085389
36	1	0	-0.664105	-3.751159	-0.146464
37	1	0	-0.428273	-2.780692	-1.609797
38	6	0	-3.331936	2.113674	-0.477325
39	1	0	-1.703909	1.804514	-1.853250
40	1	0	-2.985600	0.604801	-1.991020
41	1	0	-2.748903	2.616251	0.301815
42	1	0	-3.680704	2.891192	-1.175360
43	6	0	-4.527474	1.430973	0.116610
44	1	0	-5.223103	0.983252	-0.596429
45	6	0	-4.811361	1.366540	1.419462
46	1	0	-4.162623	1.820857	2.166372
47	1	0	-5.712880	0.882080	1.786232

HF=-2307.5841398

1	2	3
A	A	A

Frequencies --	-66.9334			15.2718			29.9415		
Red. masses --	14.1609			4.3169			5.1160		
Frc consts --	0.0374			0.0006			0.0027		
IR Inten --	4.2585			0.0481			0.0670		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.09	-0.12	-0.02	0.00	-0.02	0.08	-0.03	-0.04	0.01
2 6	-0.07	-0.09	0.00	0.01	-0.02	0.04	-0.03	-0.05	0.02
3 6	-0.05	-0.09	0.01	-0.01	0.00	0.02	0.01	0.00	0.02
4 6	-0.04	-0.11	0.00	-0.04	0.01	0.04	0.07	0.06	0.00
5 6	-0.06	-0.13	-0.01	-0.04	0.01	0.07	0.08	0.07	-0.02
6 6	-0.08	-0.13	-0.02	-0.03	-0.01	0.09	0.03	0.02	-0.01
7 1	-0.10	-0.11	-0.03	0.01	-0.04	0.09	-0.07	-0.08	0.01
8 1	-0.04	-0.14	-0.02	-0.06	0.02	0.08	0.12	0.11	-0.03
9 1	-0.08	-0.14	-0.04	-0.03	-0.01	0.12	0.04	0.03	-0.03
10 15	0.02	-0.05	0.01	-0.05	0.04	0.01	0.12	0.11	0.00
11 1	0.13	-0.12	0.02	-0.04	0.04	0.00	0.12	0.14	-0.09
12 1	-0.06	-0.07	0.00	-0.08	0.06	0.02	0.18	0.17	0.03
13 15	-0.05	-0.02	0.00	0.05	-0.04	0.02	-0.11	-0.11	0.05
14 1	-0.06	-0.11	0.00	0.08	-0.03	0.05	-0.16	-0.17	0.00
15 1	-0.17	0.07	0.00	0.07	-0.05	0.00	-0.14	-0.11	0.14
16 16	0.12	0.09	0.00	0.02	-0.05	-0.02	-0.07	-0.08	0.02
17 16	0.05	0.12	0.00	-0.04	0.05	-0.03	0.10	0.07	0.07
18 46	0.15	0.22	0.02	0.00	0.01	-0.02	0.01	0.00	0.04
19 8	-0.03	-0.26	0.01	0.02	0.00	-0.08	0.01	0.00	0.05
20 6	-0.16	-0.18	0.01	0.02	-0.01	-0.10	0.00	0.00	0.04
21 1	-0.15	-0.05	0.07	0.02	-0.02	-0.11	0.00	0.00	0.02
22 1	-0.32	-0.27	-0.05	0.03	0.00	-0.13	0.01	0.00	0.05
23 1	-0.07	-0.15	0.03	-0.12	0.08	0.03	0.02	0.07	-0.09
24 6	-0.06	-0.12	0.04	-0.06	0.04	0.03	0.00	0.04	-0.10
25 50	-0.05	-0.05	0.00	0.01	-0.01	-0.04	-0.02	0.01	-0.06
26 1	-0.06	-0.11	0.03	-0.05	0.03	0.10	-0.01	0.03	-0.09
27 1	-0.06	-0.12	0.07	-0.06	0.04	0.01	0.00	0.04	-0.14
28 8	-0.11	-0.07	-0.04	-0.03	0.02	0.02	0.00	0.01	-0.01
29 6	0.00	-0.02	0.01	0.13	-0.11	-0.02	-0.02	-0.03	-0.06
30 6	-0.03	-0.03	0.01	-0.02	0.02	-0.19	-0.02	0.01	-0.06
31 6	-0.10	-0.09	-0.05	-0.06	0.04	0.08	0.01	0.04	0.02
32 1	0.09	-0.04	0.06	0.03	-0.09	-0.07	0.33	-0.13	-0.02
33 1	-0.01	0.07	-0.01	0.20	-0.25	-0.06	-0.12	0.30	-0.06
34 1	-0.05	-0.08	0.00	0.22	-0.03	0.08	-0.26	-0.30	-0.11
35 1	-0.04	-0.03	0.04	-0.01	-0.06	-0.14	-0.02	0.02	-0.08
36 1	-0.02	-0.04	-0.01	-0.04	-0.02	-0.34	-0.01	0.01	-0.04
37 1	0.00	-0.01	0.01	-0.02	0.17	-0.20	-0.04	-0.02	-0.06
38 6	-0.08	-0.06	-0.06	-0.02	0.02	0.14	-0.01	0.00	0.05
39 1	-0.10	-0.11	-0.07	-0.08	0.05	0.06	0.01	0.07	0.06
40 1	-0.13	-0.08	-0.04	-0.09	0.06	0.09	0.02	0.07	-0.01
41 1	-0.06	-0.05	-0.07	0.02	0.00	0.13	-0.02	-0.05	0.09
42 1	-0.09	-0.07	-0.07	-0.05	0.04	0.18	0.01	0.04	0.09
43 6	-0.07	-0.03	-0.01	0.01	0.01	0.18	-0.02	-0.03	-0.02
44 1	-0.09	-0.04	0.01	-0.03	0.03	0.20	-0.02	0.03	-0.07
45 6	-0.04	-0.02	-0.01	0.07	-0.04	0.19	-0.04	-0.13	-0.03
46 1	-0.01	-0.01	-0.03	0.11	-0.06	0.17	-0.05	-0.20	0.02
47 1	-0.03	-0.01	0.02	0.09	-0.05	0.22	-0.05	-0.15	-0.08

thermodynamics:
Sum of electronic and zero-point Energies= -2307.226683

Sum of electronic and thermal Enthalpies= -2307.193827

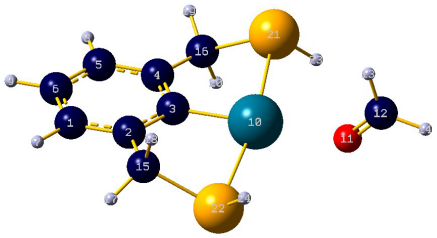
Sum of electronic and thermal Free Energies= -2307.294295

Total free energy in solution:
with all non electrostatic terms (a.u.) = -2307.614188

IV. Comparison with literature complexes

Se~C~*Se* complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016329	0.052567	0.029902
2	6	0	0.035164	0.064217	1.429538
3	6	0	1.263832	-0.016458	2.114499
4	6	0	2.460972	-0.089930	1.375335
5	6	0	2.418994	-0.054579	-0.023360
6	6	0	1.202420	0.005772	-0.694067
7	1	0	-0.936266	0.088525	-0.493037
8	1	0	3.347739	-0.083473	-0.587960
9	1	0	1.178807	0.015479	-1.779430
10	46	0	1.303322	-0.004389	4.101478
11	8	0	1.319756	-0.022582	6.327128
12	6	0	1.340018	0.882953	7.143807
13	1	0	1.371119	1.941899	6.842199
14	1	0	1.328298	0.650374	8.218733
15	6	0	-1.257424	0.185563	2.171226
16	6	0	3.783975	-0.235075	2.055215
17	1	0	-2.106441	-0.246912	1.638229
18	1	0	-1.490227	1.216848	2.451250
19	1	0	4.612605	0.202314	1.494964
20	1	0	4.020193	-1.273274	2.305356
21	34	0	3.679232	0.722909	3.834263
22	34	0	-1.053386	-0.812717	3.916457
23	1	0	4.349565	-0.344088	4.639161
24	1	0	-1.756867	0.193605	4.770804

HF=-569.6996904

	1			2			3		
	A			A			A		
Frequencies --	38.8934			45.0349			62.2374		
Red. masses --	2.5932			6.4322			4.2987		
Frc consts --	0.0023			0.0077			0.0098		
IR Inten --	10.8002			1.9207			0.4922		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.01	-0.01	-0.01	-0.03	0.11	0.01	0.01	0.15	0.04
2 6	0.00	-0.02	-0.01	-0.02	0.03	0.02	0.01	0.12	0.04
3 6	0.00	0.00	0.00	-0.02	0.01	0.00	0.00	-0.01	0.03
4 6	0.00	0.01	0.01	-0.02	0.06	-0.01	-0.01	-0.13	0.04
5 6	0.02	0.01	0.01	-0.03	0.14	-0.01	0.00	-0.12	0.04
6 6	0.02	0.00	0.00	-0.04	0.17	0.00	0.00	0.03	0.04
7 1	0.02	-0.02	-0.02	-0.04	0.13	0.02	0.01	0.26	0.04
8 1	0.02	0.02	0.02	-0.04	0.18	-0.02	0.00	-0.21	0.04
9 1	0.03	0.00	0.00	-0.05	0.24	0.00	0.01	0.04	0.04
10 46	-0.02	0.00	0.00	-0.01	0.03	0.00	0.00	0.00	0.03
11 8	-0.09	0.02	0.00	-0.05	0.23	0.00	-0.02	0.03	0.03
12 6	0.34	0.02	-0.01	-0.06	0.35	-0.13	0.03	0.04	0.02
13 1	0.91	0.00	-0.02	-0.04	0.30	-0.29	0.10	0.03	0.00
14 1	0.16	0.04	-0.01	-0.10	0.51	-0.10	-0.01	0.05	0.02
15 6	-0.01	-0.03	-0.02	-0.02	-0.05	0.03	0.03	0.19	0.08
16 6	0.00	0.02	0.02	-0.02	0.00	-0.04	-0.04	-0.23	0.08
17 1	0.00	-0.04	-0.03	-0.01	-0.06	0.02	-0.03	0.35	0.05

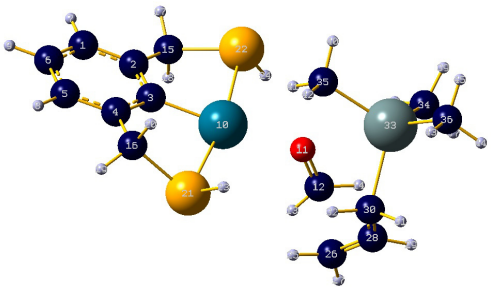
18	1	-0.02	-0.03	-0.04	-0.06	-0.07	0.07	0.16	0.18	0.22
19	1	0.00	0.03	0.02	-0.02	0.03	-0.02	0.03	-0.42	0.05
20	1	0.01	0.02	0.01	-0.02	-0.02	-0.11	-0.20	-0.22	0.25
21	34	-0.02	0.00	0.02	0.04	-0.12	0.03	-0.02	0.05	-0.06
22	34	-0.01	-0.01	-0.02	0.04	-0.10	-0.01	0.02	-0.07	-0.06
23	1	-0.02	-0.01	0.02	-0.07	-0.23	-0.03	0.05	0.21	0.09
24	1	-0.02	-0.01	-0.03	-0.04	-0.18	0.03	-0.04	-0.22	0.08

thermodynamics:
Sum of electronic and zero-point Energies= -569.525806

Sum of electronic and thermal Enthalpies= -569.509423

Sum of electronic and thermal Free Energies= -569.570916
Total free energy in solution:
with all non electrostatic terms (a.u.) = -569.738641

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{B2B3}**.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.156536	0.119623	-0.232310
2	6	0	-0.044723	0.127770	1.162750
3	6	0	1.226523	0.097851	1.773270
4	6	0	2.371045	0.083764	0.949922
5	6	0	2.239019	0.121073	-0.442968
6	6	0	0.980066	0.127474	-1.033437
7	1	0	-1.142098	0.117943	-0.691945
8	1	0	3.129408	0.134686	-1.067134
9	1	0	0.884966	0.138909	-2.114986
10	46	0	1.394568	0.093295	3.760644
11	8	0	1.459368	0.027068	5.928471
12	6	0	1.381704	1.035358	6.685447
13	1	0	1.311081	2.046188	6.262805
14	1	0	0.936504	0.907072	7.678024
15	6	0	-1.293181	0.199668	1.984385
16	6	0	3.742575	-0.002077	1.539095
17	1	0	-2.154660	-0.273219	1.508497
18	1	0	-1.552998	1.223712	2.268039
19	1	0	4.509196	0.487303	0.934977
20	1	0	4.048186	-1.030576	1.752155
21	34	0	3.705551	0.915502	3.341653
22	34	0	-0.942640	-0.763552	3.724616
23	1	0	4.474062	-0.135563	4.075466
24	1	0	-1.595587	0.245584	4.613636
25	1	0	3.776977	1.701233	6.465569
26	6	0	3.299041	1.622159	7.439726
27	1	0	2.971046	2.558343	7.884543
28	6	0	3.570824	0.549738	8.252268
29	1	0	3.231119	0.616115	9.288196
30	6	0	4.196458	-0.693722	7.866400
31	1	0	4.846460	-1.074407	8.662298
32	1	0	4.752052	-0.635242	6.926436

33	50	0	2.824642	-2.487305	7.701883
34	6	0	0.875867	-2.099167	8.512957
35	6	0	2.825692	-3.134232	5.654944
36	6	0	3.862180	-3.917111	8.924608
37	1	0	0.938960	-1.585676	9.477399
38	1	0	0.284568	-1.497339	7.819103
39	1	0	0.360425	-3.051359	8.675930
40	1	0	2.271931	-4.074321	5.560711
41	1	0	2.352465	-2.384277	5.014218
42	1	0	3.850174	-3.311434	5.311523
43	1	0	4.881753	-4.076660	8.559335
44	1	0	3.914957	-3.578710	9.964417
45	1	0	3.340571	-4.879719	8.907559

HF=-810.0525161

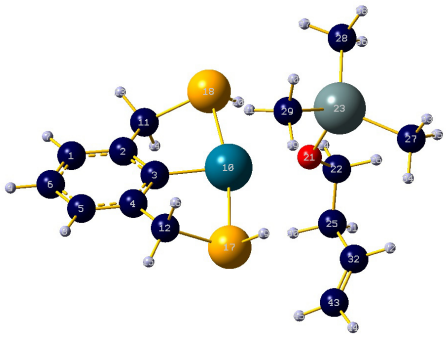
		1			2			3		
		A			A			A		
Frequencies --		-159.0793			8.7785			15.6086		
Red. masses --		7.5628			7.5939			6.9579		
Frc consts --		0.1128			0.0003			0.0010		
IR Inten --		271.8348			0.1912			0.0094		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	-0.01	-0.03	-0.11	0.02	-0.06	0.19	-0.02
2	6	0.00	0.00	-0.01	-0.01	-0.08	0.02	-0.03	0.10	-0.02
3	6	0.00	0.00	-0.02	0.00	-0.01	0.00	-0.03	0.06	-0.04
4	6	0.01	0.00	-0.01	-0.01	0.04	-0.02	-0.04	0.11	-0.06
5	6	0.01	0.00	-0.01	-0.03	0.01	-0.02	-0.06	0.19	-0.06
6	6	0.01	0.00	-0.01	-0.04	-0.07	0.00	-0.07	0.24	-0.04
7	1	0.01	0.00	-0.01	-0.04	-0.17	0.04	-0.06	0.22	-0.01
8	1	0.01	0.00	-0.01	-0.05	0.04	-0.03	-0.07	0.23	-0.07
9	1	0.01	0.00	-0.01	-0.06	-0.09	0.00	-0.09	0.30	-0.04
10	46	-0.01	0.00	-0.03	0.04	0.03	0.00	0.00	-0.02	-0.05
11	8	-0.17	0.04	0.00	0.05	0.05	0.00	0.02	-0.07	-0.05
12	6	-0.32	-0.08	-0.03	0.11	0.06	0.00	0.01	-0.06	-0.05
13	1	0.06	0.01	0.12	0.16	0.06	0.00	-0.01	-0.07	-0.06
14	1	0.04	-0.13	0.11	0.12	0.08	0.00	0.01	-0.06	-0.05
15	6	0.00	0.00	-0.01	0.00	-0.13	0.04	-0.02	0.05	0.00
16	6	0.00	0.00	0.00	0.00	0.12	-0.04	-0.03	0.06	-0.09
17	1	0.00	0.01	-0.02	0.02	-0.18	0.06	-0.03	0.08	-0.01
18	1	0.00	0.00	-0.01	-0.05	-0.14	0.02	-0.02	0.04	0.06
19	1	0.01	-0.01	0.01	-0.03	0.15	-0.06	-0.03	0.09	-0.07
20	1	0.00	-0.01	0.00	0.06	0.14	-0.03	-0.04	0.05	-0.14
21	34	0.00	0.00	0.00	-0.01	0.15	-0.06	0.01	-0.03	-0.04
22	34	-0.01	-0.01	-0.02	0.08	-0.08	0.05	0.01	-0.04	-0.06
23	1	-0.02	0.00	0.02	0.06	0.20	-0.05	0.00	-0.07	-0.10
24	1	-0.02	-0.01	-0.02	0.05	-0.10	0.04	0.01	-0.10	0.01
25	1	0.29	0.18	0.17	0.14	-0.08	-0.03	0.00	-0.07	-0.08
26	6	0.50	0.23	0.27	0.15	-0.06	-0.03	0.00	-0.03	-0.08
27	1	0.28	0.18	0.21	0.22	-0.04	-0.02	0.00	-0.02	-0.11
28	6	0.05	0.07	0.07	0.11	-0.07	-0.03	0.01	0.00	-0.03
29	1	-0.04	-0.02	0.05	0.14	-0.05	-0.02	0.02	0.04	-0.03
30	6	-0.08	-0.06	-0.04	0.03	-0.11	-0.04	0.02	-0.01	0.01
31	1	0.09	0.06	-0.11	0.04	-0.14	-0.06	0.03	0.03	0.02
32	1	-0.08	0.05	-0.04	0.01	-0.14	-0.06	0.00	-0.05	0.00
33	50	0.03	0.00	0.02	-0.08	-0.03	0.01	0.02	-0.02	0.12
34	6	0.00	-0.03	-0.01	-0.05	0.10	0.02	0.01	0.04	0.08
35	6	-0.05	-0.02	0.01	-0.14	-0.06	0.02	0.00	-0.11	0.15
36	6	-0.05	-0.08	-0.01	-0.16	-0.07	0.03	0.01	0.05	0.20
37	1	-0.01	0.01	-0.03	-0.01	0.12	0.01	0.01	0.11	0.05
38	1	-0.06	-0.09	-0.01	-0.02	0.12	0.01	0.01	-0.02	0.04
39	1	0.02	-0.04	0.05	-0.10	0.13	0.05	0.01	0.05	0.15
40	1	-0.06	-0.01	0.00	-0.25	0.00	0.04	0.00	-0.12	0.19
41	1	-0.03	-0.02	-0.01	-0.05	-0.02	0.01	0.00	-0.14	0.12
42	1	-0.05	-0.04	0.00	-0.16	-0.18	0.03	0.00	-0.13	0.15
43	1	-0.05	-0.09	-0.01	-0.18	-0.16	0.01	0.00	0.01	0.20
44	1	-0.03	-0.08	-0.01	-0.10	-0.04	0.02	0.02	0.12	0.18
45	1	-0.05	-0.07	-0.01	-0.23	-0.03	0.08	0.00	0.05	0.27

```
thermodynamics:
Sum of electronic and zero-point Energies=           -809.696715

Sum of electronic and thermal Enthalpies=            -809.667442

Sum of electronic and thermal Free Energies=         -809.761201
  Total free energy in solution:
  with all non electrostatic terms            (a.u.) =    -810.069547
```

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B3.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.892323	0.907948	0.037590
2	6	0	0.695220	0.995312	1.420465
3	6	0	1.261796	0.031753	2.279513
4	6	0	2.043533	-1.000528	1.720539
5	6	0	2.263313	-1.045773	0.338973
6	6	0	1.682335	-0.102059	-0.501200
7	1	0	0.430113	1.641799	-0.618466
8	1	0	2.887323	-1.831824	-0.079659
9	1	0	1.843918	-0.153789	-1.573649
10	46	0	0.935758	0.094250	4.245943
11	6	0	-0.102832	2.135573	1.966820
12	6	0	2.631290	-2.067521	2.589923
13	1	0	-0.864100	2.506104	1.277446
14	1	0	0.520431	2.969114	2.303395
15	1	0	3.556240	-2.490818	2.192648
16	1	0	1.926036	-2.876003	2.803511
17	34	0	3.047522	-1.215140	4.372304
18	34	0	-1.049672	1.479293	3.629401
19	1	0	2.608705	-2.354888	5.231212
20	1	0	-0.793673	2.691877	4.466042
21	8	0	0.521989	0.040630	6.397441
22	6	0	0.806504	1.205692	7.177824
23	50	0	-0.852665	-1.300264	7.087309
24	1	0	0.209819	2.052051	6.807790
25	6	0	2.284894	1.574269	7.160610
26	1	0	0.497801	1.023837	8.218259
27	6	0	-0.165786	-1.817708	9.043553
28	6	0	-2.717404	-0.254151	7.060660
29	6	0	-0.707755	-2.880594	5.657147
30	1	0	2.605200	1.798233	6.133740
31	1	0	2.377596	2.514924	7.726480
32	6	0	3.177366	0.535159	7.776060
33	1	0	-0.730150	-2.682587	9.408230
34	1	0	0.894245	-2.087044	9.020430
35	1	0	-0.309146	-0.998233	9.753539
36	1	0	-2.647876	0.681887	7.623082
37	1	0	-3.032628	-0.033448	6.036497
38	1	0	-3.491505	-0.871607	7.528532

39	1	0	0.183347	-3.490748	5.833480
40	1	0	-1.585279	-3.530530	5.741321
41	1	0	-0.677096	-2.482706	4.637783
42	1	0	2.818378	0.089957	8.706187
43	6	0	4.373796	0.174723	7.306885
44	1	0	4.996797	-0.546521	7.829138
45	1	0	4.793962	0.617800	6.406020

HF=-810.1150422

	1			2			3		
	A			A			A		
Frequencies --	20.5309			21.4967			25.0752		
Red. masses --	3.8699			5.0675			4.6010		
Frc consts --	0.0010			0.0014			0.0017		
IR Inten --	0.0243			0.0409			0.0173		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.06	-0.01	0.02	0.01	-0.04	0.01	0.08	0.08	0.00
2 6	-0.04	-0.01	0.02	0.03	-0.01	0.01	0.05	0.06	-0.01
3 6	-0.01	0.00	0.02	0.00	-0.02	0.02	0.00	0.02	-0.01
4 6	-0.02	0.00	0.00	-0.05	-0.05	0.03	-0.01	0.01	-0.02
5 6	-0.05	-0.01	0.00	-0.06	-0.09	0.03	0.02	0.03	-0.01
6 6	-0.07	-0.01	0.01	-0.04	-0.08	0.02	0.07	0.07	-0.01
7 1	-0.08	-0.01	0.03	0.03	-0.03	0.01	0.12	0.11	0.00
8 1	-0.06	0.00	-0.01	-0.10	-0.12	0.04	0.01	0.03	-0.01
9 1	-0.09	-0.01	0.00	-0.05	-0.10	0.02	0.09	0.09	0.00
10 46	0.02	-0.01	0.02	0.00	0.01	0.02	-0.03	0.00	-0.02
11 6	-0.03	-0.01	0.04	0.08	0.03	0.01	0.07	0.07	0.00
12 6	0.00	0.00	-0.01	-0.07	-0.06	0.04	-0.06	-0.02	-0.02
13 1	-0.04	-0.01	0.05	0.09	0.06	0.01	0.10	0.10	-0.01
14 1	-0.02	-0.01	0.03	0.11	0.01	0.00	0.08	0.04	0.04
15 1	0.00	0.01	-0.02	-0.09	-0.10	0.04	-0.07	-0.05	-0.01
16 1	0.01	0.00	0.01	-0.09	-0.03	0.07	-0.09	0.00	-0.04
17 34	0.03	0.01	-0.02	-0.02	-0.03	0.02	-0.06	-0.06	-0.01
18 34	0.00	-0.01	0.05	0.06	0.09	0.02	0.01	0.05	-0.04
19 1	0.07	0.01	0.00	-0.04	-0.01	0.05	-0.10	-0.05	-0.03
20 1	0.01	-0.01	0.05	0.11	0.08	0.00	0.00	0.03	-0.01
21 8	0.04	-0.03	0.03	-0.01	-0.02	0.02	-0.03	0.02	-0.02
22 6	0.05	-0.03	0.04	-0.06	-0.02	0.04	-0.03	0.03	-0.04
23 50	-0.03	0.01	-0.03	0.00	-0.05	-0.03	0.04	-0.02	0.04
24 1	0.03	-0.04	0.07	-0.15	-0.05	0.10	-0.02	0.03	-0.07
25 6	0.04	-0.02	0.00	-0.09	0.11	-0.03	-0.03	0.02	-0.03
26 1	0.08	-0.06	0.04	0.01	-0.08	0.05	-0.05	0.06	-0.04
27 6	-0.21	0.12	0.06	0.01	-0.10	-0.04	0.02	0.16	0.10
28 6	-0.03	0.00	-0.26	-0.01	-0.06	0.00	-0.03	-0.15	-0.08
29 6	0.12	-0.06	0.06	0.01	-0.01	-0.07	0.18	-0.11	0.15
30 1	0.01	0.01	0.00	-0.17	0.14	-0.05	-0.01	-0.02	-0.03
31 1	0.04	-0.02	0.02	-0.14	0.11	-0.03	-0.03	0.03	-0.06
32 6	0.07	-0.02	-0.04	0.03	0.17	-0.10	-0.05	0.02	0.01
33 1	-0.23	0.12	0.04	0.11	-0.20	-0.12	-0.01	0.21	0.18
34 1	-0.20	0.15	0.19	0.04	0.02	-0.04	0.01	0.12	0.13
35 1	-0.32	0.15	0.01	-0.10	-0.17	0.01	0.04	0.23	0.01
36 1	-0.07	0.05	-0.34	-0.02	-0.09	0.05	-0.12	-0.13	-0.12
37 1	0.04	-0.10	-0.30	0.01	-0.01	0.00	0.00	-0.22	-0.11
38 1	-0.06	0.04	-0.25	-0.01	-0.09	-0.05	-0.01	-0.19	-0.09
39 1	0.16	0.01	0.12	-0.01	-0.03	-0.07	0.26	0.01	0.16
40 1	0.16	-0.12	0.08	-0.01	0.01	-0.11	0.27	-0.22	0.24
41 1	0.12	-0.12	0.04	0.03	0.02	-0.06	0.08	-0.18	0.12
42 1	0.09	-0.05	-0.05	0.12	0.14	-0.08	-0.06	0.07	0.03
43 6	0.07	0.02	-0.07	0.03	0.27	-0.17	-0.06	-0.03	0.02
44 1	0.10	0.02	-0.10	0.12	0.32	-0.22	-0.08	-0.02	0.05
45 1	0.05	0.06	-0.06	-0.07	0.31	-0.20	-0.05	-0.08	0.00

thermodynamics:

Sum of electronic and zero-point Energies= -809.756196

Sum of electronic and thermal Enthalpies= -809.726798

Sum of electronic and thermal Free Energies= -809.820107

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Total free energy in solution:
 with all non electrostatic terms            (a.u.) =    -810.132451
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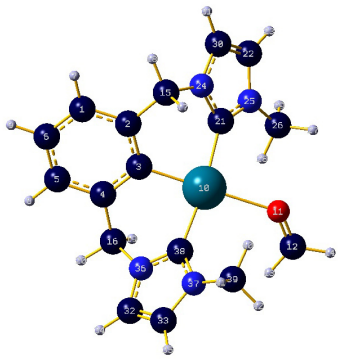
biscarbene complex

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B2.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003531	0.000475	0.028064
2	6	0	-0.001869	-0.006680	1.426553
3	6	0	1.206713	-0.003410	2.139298
4	6	0	2.413997	0.003320	1.422070
5	6	0	2.404750	0.016268	0.023972
6	6	0	1.202789	0.014981	-0.676442
7	1	0	-0.940388	-0.000604	-0.513141
8	1	0	3.346884	0.021037	-0.520398
9	1	0	1.200860	0.023081	-1.762351
10	46	0	1.217883	-0.001730	4.136403
11	8	0	1.237998	0.048844	6.392041
12	6	0	2.203165	0.112286	7.132234
13	1	0	3.235116	0.103192	6.746668
14	1	0	2.060593	0.179664	8.221999
15	6	0	-1.321664	0.000562	2.159853
16	6	0	3.736339	-0.039076	2.152001
17	1	0	-1.491450	-0.944838	2.688044
18	1	0	-2.153387	0.148180	1.466866
19	1	0	3.920122	0.887337	2.707904
20	1	0	4.566135	-0.180588	1.455467
21	6	0	-0.365400	1.293905	4.024323
22	6	0	-1.946967	2.885783	4.245342
23	1	0	-2.409892	3.772559	4.650996
24	7	0	-1.365317	1.086449	3.141380
25	7	0	-0.729050	2.411738	4.698764
26	6	0	0.041436	3.047134	5.754144
27	1	0	-0.311441	2.727372	6.738975
28	1	0	1.091067	2.779154	5.632559
29	1	0	-0.056369	4.131844	5.669536
30	6	0	-2.347597	2.046705	3.256037
31	1	0	-3.229411	2.057452	2.633709
32	6	0	4.665202	-2.192340	3.140458
33	6	0	4.219915	-3.055716	4.089720
34	1	0	5.535559	-2.231361	2.503070
35	1	0	4.622613	-3.996106	4.434762
36	7	0	3.757849	-1.155188	3.102260
37	7	0	3.049325	-2.518489	4.597098
38	6	0	2.758146	-1.340691	3.990235
39	6	0	2.209808	-3.190502	5.576155

40	1	0	1.293602	-2.614250	5.705080
41	1	0	1.950213	-4.190055	5.217257
42	1	0	2.730424	-3.279923	6.534658

HF=-1079.7111038

	1			2			3		
	A			A			A		
Frequencies --	39.9809			52.7802			59.8671		
Red. masses --	4.8075			3.9467			3.3826		
Frc consts --	0.0045			0.0065			0.0071		
IR Inten --	0.9591			1.4686			7.3342		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.05	0.03	-0.02	0.01	-0.07	0.05	-0.01	0.12	0.00
2 6	0.04	0.02	-0.02	0.02	-0.06	0.05	0.00	0.02	0.00
3 6	0.04	0.01	-0.01	0.02	0.01	0.04	0.00	-0.02	0.00
4 6	0.04	-0.02	0.00	0.02	0.06	0.04	0.00	0.01	0.00
5 6	0.05	-0.01	0.00	0.01	0.06	0.04	-0.01	0.12	0.00
6 6	0.06	0.02	-0.01	0.01	0.00	0.05	-0.01	0.18	0.00
7 1	0.06	0.05	-0.03	0.01	-0.12	0.05	-0.01	0.16	0.01
8 1	0.06	-0.03	0.00	0.01	0.11	0.04	-0.01	0.15	-0.01
9 1	0.06	0.03	-0.01	0.01	0.00	0.05	-0.01	0.27	0.00
10 46	0.03	0.05	-0.01	0.02	0.02	0.04	0.00	-0.04	0.00
11 8	0.12	0.14	-0.01	0.01	0.04	0.04	-0.02	-0.06	0.00
12 6	0.17	0.12	-0.08	0.00	0.00	0.05	-0.06	0.30	0.02
13 1	0.14	0.02	-0.14	0.00	-0.05	0.06	-0.04	0.71	0.04
14 1	0.24	0.20	-0.07	-0.01	0.01	0.05	-0.10	0.20	0.02
15 6	0.04	0.00	-0.04	0.03	-0.12	0.07	0.01	-0.04	0.02
16 6	0.04	-0.06	0.00	0.01	0.08	0.06	0.00	-0.05	-0.02
17 1	0.04	-0.02	-0.06	0.09	-0.10	0.11	0.05	-0.05	0.01
18 1	0.05	0.01	-0.05	0.00	-0.19	0.08	-0.01	-0.06	0.03
19 1	0.08	-0.07	0.00	-0.03	0.06	0.10	0.05	-0.06	-0.01
20 1	0.04	-0.09	0.00	0.03	0.13	0.07	-0.01	-0.07	-0.03
21 6	-0.01	0.00	0.00	0.00	0.00	0.01	0.00	-0.03	0.00
22 6	-0.13	-0.13	0.09	-0.01	0.00	-0.10	0.01	-0.01	-0.02
23 1	-0.19	-0.18	0.14	-0.02	0.02	-0.16	0.02	0.00	-0.04
24 7	0.00	-0.03	-0.01	-0.01	-0.08	0.03	-0.01	-0.05	0.02
25 7	-0.09	-0.06	0.06	-0.01	0.04	-0.07	0.02	-0.01	-0.02
26 6	-0.14	-0.06	0.09	0.00	0.14	-0.14	0.04	0.03	-0.07
27 1	-0.06	-0.21	0.07	-0.07	0.33	-0.11	0.06	0.09	-0.05
28 1	-0.11	0.10	0.03	-0.02	0.01	-0.05	0.04	0.02	-0.08
29 1	-0.30	-0.07	0.21	0.12	0.13	-0.32	0.06	0.03	-0.12
30 6	-0.07	-0.11	0.05	-0.01	-0.08	-0.04	0.00	-0.04	0.01
31 1	-0.08	-0.14	0.06	-0.02	-0.13	-0.03	-0.01	-0.05	0.02
32 6	-0.08	-0.13	-0.01	-0.05	-0.02	-0.10	-0.02	-0.06	-0.01
33 6	-0.13	-0.10	-0.01	-0.08	-0.08	-0.16	0.00	-0.03	0.01
34 1	-0.09	-0.18	-0.02	-0.06	-0.02	-0.11	-0.03	-0.07	-0.03
35 1	-0.19	-0.12	-0.02	-0.13	-0.13	-0.24	0.00	-0.03	0.03
36 7	-0.01	-0.06	0.00	0.01	0.04	0.01	-0.02	-0.06	-0.03
37 7	-0.09	-0.02	0.00	-0.05	-0.05	-0.10	0.01	-0.02	0.02
38 6	-0.01	0.00	0.01	0.01	0.01	0.01	0.00	-0.04	0.00
39 6	-0.13	0.04	0.01	-0.07	-0.09	-0.14	0.04	0.02	0.07
40 1	-0.08	0.11	0.02	-0.01	-0.01	-0.04	0.04	0.02	0.08
41 1	-0.20	0.06	0.01	-0.19	-0.02	-0.25	0.03	0.00	0.13
42 1	-0.12	0.00	0.00	-0.04	-0.25	-0.17	0.07	0.06	0.06

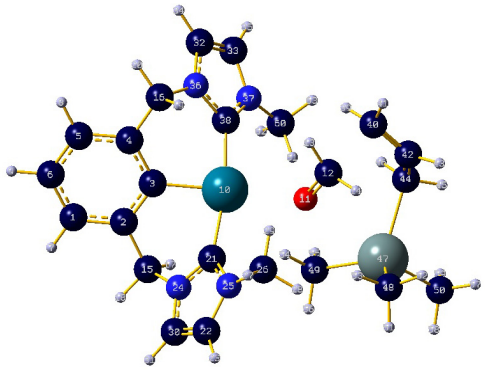
thermodynamics:
Sum of electronic and zero-point Energies= -1079.369624

Sum of electronic and thermal Enthalpies= -1079.346737

Sum of electronic and thermal Free Energies= -1079.420567

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1079.745267

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **TS_{B2B3}.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.055957	-0.049341	0.039013
2	6	0	-0.020833	-0.002247	1.435979
3	6	0	1.204739	-0.001977	2.119980
4	6	0	2.389592	-0.050770	1.367484
5	6	0	2.345120	-0.090405	-0.029082
6	6	0	1.124222	-0.090348	-0.697246
7	1	0	-1.014326	-0.047903	-0.476702
8	1	0	3.272272	-0.129208	-0.597743
9	1	0	1.092850	-0.123790	-1.782360
10	46	0	1.263956	0.066816	4.121321
11	8	0	1.299452	0.234424	6.351262
12	6	0	2.336434	0.717170	6.912295
13	1	0	3.244895	0.883910	6.315315
14	1	0	2.196684	1.447425	7.721681
15	6	0	-1.311597	0.087666	2.215983
16	6	0	3.722005	-0.116326	2.078329
17	1	0	-1.482321	-0.812793	2.816729
18	1	0	-2.169048	0.214160	1.550327
19	1	0	3.933199	0.808006	2.627261
20	1	0	4.542050	-0.286246	1.376277
21	6	0	-0.235055	1.456034	3.954387
22	6	0	-1.661361	3.204948	4.007503
23	1	0	-2.030629	4.172266	4.312922
24	7	0	-1.275332	1.241531	3.117847
25	7	0	-0.479693	2.674575	4.495651
26	6	0	0.404262	3.388016	5.399278
27	1	0	0.603227	4.388361	5.004928
28	1	0	-0.044509	3.473856	6.392899
29	1	0	1.341589	2.839123	5.467150
30	6	0	-2.162204	2.297348	3.131459
31	1	0	-3.057045	2.315962	2.528101
32	6	0	4.530897	-2.338189	3.017649
33	6	0	4.040945	-3.188537	3.955931
34	1	0	5.381713	-2.427199	2.359305
35	1	0	4.374434	-4.166907	4.267357
36	7	0	3.714509	-1.226428	3.035866
37	7	0	2.936281	-2.567308	4.514118
38	6	0	2.725866	-1.353042	3.948276
39	1	0	3.438012	-1.387170	7.211697
40	6	0	3.337865	-0.650706	8.004498
41	1	0	4.230806	-0.065888	8.213927
42	6	0	2.454103	-0.882192	9.041496
43	1	0	2.551212	-0.245619	9.923581
44	6	0	1.346475	-1.794255	9.038548
45	1	0	1.117229	-2.174857	10.038360
46	1	0	1.429601	-2.610124	8.318232
47	50	0	-0.676155	-0.823296	8.633962
48	6	0	-0.616008	1.306118	8.877124
49	6	0	-1.502414	-1.531968	6.786553

50	6	0	-1.786594	-1.678276	10.267705
51	1	0	-1.637389	1.681582	8.998749
52	1	0	-0.045049	1.591545	9.765951
53	1	0	-0.171058	1.765829	7.993221
54	1	0	-0.966774	-1.106125	5.934625
55	1	0	-1.459067	-2.624762	6.739605
56	1	0	-2.555700	-1.235849	6.730718
57	1	0	-1.378356	-1.356530	11.231429
58	1	0	-2.833241	-1.358911	10.220434
59	1	0	-1.765043	-2.772250	10.229704
60	6	0	2.028247	-3.205672	5.449502
61	1	0	1.376991	-2.438752	5.869005
62	1	0	1.420063	-3.956091	4.934833
63	1	0	2.596007	-3.691962	6.247842

HF=-1320.0531492

		1			2			3		
		A			A			A		
Frequencies --		-241.4158			17.0313			24.2609		
Red. masses --		8.5479			6.0873			4.9872		
Frc consts --		0.2935			0.0010			0.0017		
IR Inten --		363.1914			0.4433			0.8028		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.12	-0.06	0.09	-0.03	-0.02	0.00
2	6	0.00	0.00	0.00	-0.07	-0.04	0.09	-0.02	0.01	0.00
3	6	0.00	0.00	-0.01	-0.04	-0.02	0.04	-0.01	0.00	-0.01
4	6	0.00	0.00	0.00	-0.07	-0.03	0.00	-0.02	-0.05	-0.02
5	6	0.00	0.00	0.00	-0.12	-0.05	0.00	-0.03	-0.09	-0.02
6	6	0.00	0.00	0.00	-0.15	-0.07	0.04	-0.04	-0.08	-0.01
7	1	0.00	0.00	0.00	-0.14	-0.08	0.13	-0.04	-0.01	0.01
8	1	0.00	0.00	0.00	-0.15	-0.06	-0.04	-0.04	-0.12	-0.03
9	1	0.00	0.00	0.00	-0.19	-0.09	0.05	-0.05	-0.11	-0.01
10	46	0.00	0.00	-0.03	0.03	-0.01	0.04	0.00	0.03	-0.01
11	8	-0.01	0.15	-0.07	0.05	-0.01	0.04	-0.03	0.03	-0.02
12	6	-0.20	0.29	-0.16	0.03	0.00	0.05	-0.07	0.09	0.00
13	1	0.03	-0.06	0.11	0.05	-0.01	0.07	-0.07	0.15	0.02
14	1	-0.14	-0.06	0.15	0.02	0.01	0.04	-0.13	0.08	0.00
15	6	0.00	0.00	0.00	-0.04	-0.02	0.13	-0.01	0.07	0.00
16	6	0.00	0.00	0.00	-0.04	0.00	-0.05	-0.02	-0.06	-0.03
17	1	0.00	0.00	0.00	-0.02	-0.01	0.16	-0.04	0.09	0.02
18	1	0.00	0.00	0.00	-0.07	-0.03	0.16	-0.01	0.09	0.00
19	1	0.01	0.00	-0.01	-0.04	0.01	-0.07	0.00	-0.05	-0.06
20	1	0.00	0.00	0.00	-0.07	0.00	-0.08	-0.03	-0.09	-0.04
21	6	0.00	0.01	-0.02	0.03	0.00	0.07	0.04	0.07	-0.03
22	6	-0.01	0.00	0.00	0.05	0.01	0.09	0.11	0.12	-0.06
23	1	-0.02	-0.01	0.00	0.07	0.02	0.09	0.14	0.14	-0.07
24	7	0.00	0.00	-0.01	0.00	-0.01	0.11	0.03	0.09	-0.02
25	7	0.00	0.01	-0.01	0.06	0.01	0.06	0.09	0.08	-0.05
26	6	-0.01	0.03	-0.02	0.11	0.02	0.00	0.11	0.06	-0.05
27	1	-0.11	0.06	0.02	0.12	0.00	-0.04	0.06	0.08	-0.01
28	1	0.05	-0.06	0.01	0.15	0.06	0.02	0.15	-0.01	-0.02
29	1	0.05	0.11	-0.12	0.10	0.00	-0.02	0.13	0.08	-0.12
30	6	-0.01	0.00	0.00	0.01	0.00	0.13	0.07	0.12	-0.04
31	1	-0.01	-0.01	0.01	-0.01	0.00	0.16	0.07	0.15	-0.04
32	6	0.00	0.00	0.00	0.03	0.03	-0.05	-0.03	-0.04	0.02
33	6	0.00	0.00	0.00	0.08	0.04	-0.02	-0.03	0.00	0.05
34	1	0.01	0.00	0.01	0.01	0.04	-0.07	-0.04	-0.06	0.02
35	1	0.00	0.01	0.01	0.12	0.05	-0.01	-0.03	0.00	0.08
36	7	0.00	0.00	0.00	0.01	0.01	-0.04	-0.02	-0.03	-0.01
37	7	0.00	0.00	0.00	0.09	0.02	0.01	-0.02	0.02	0.04
38	6	0.00	-0.01	-0.01	0.04	0.01	0.00	-0.02	0.00	0.00
39	1	0.17	-0.13	0.11	0.05	0.01	0.11	0.03	0.15	0.03
40	6	0.38	-0.39	0.36	0.01	0.01	0.10	-0.01	0.16	0.02
41	1	0.25	-0.13	0.17	0.00	0.02	0.14	-0.04	0.20	0.01
42	6	0.09	-0.01	0.04	-0.04	0.01	0.06	0.00	0.12	0.02
43	1	0.01	0.06	0.01	-0.08	0.01	0.06	-0.03	0.14	0.01
44	6	-0.12	0.09	-0.06	-0.04	0.01	0.00	0.05	0.05	0.04
45	1	0.07	-0.05	-0.06	-0.09	0.01	-0.01	0.08	0.06	0.04

46	1	0.03	0.04	0.00	0.00	0.01	0.01	0.10	0.05	0.05
47	50	0.01	-0.02	0.03	-0.02	0.01	-0.10	-0.01	-0.08	0.02
48	6	-0.03	0.00	-0.01	-0.04	0.01	-0.08	-0.13	-0.06	-0.05
49	6	-0.02	0.03	0.00	0.04	0.01	-0.13	0.04	-0.15	0.03
50	6	-0.08	0.03	-0.01	-0.09	0.01	-0.15	0.05	-0.11	0.04
51	1	-0.03	0.00	0.04	-0.05	0.00	-0.11	-0.15	-0.12	-0.03
52	1	0.00	0.00	-0.03	-0.07	0.01	-0.07	-0.12	0.00	-0.07
53	1	-0.09	0.06	-0.01	-0.02	0.02	-0.07	-0.18	-0.07	-0.08
54	1	-0.04	0.01	-0.03	0.07	0.01	-0.11	0.01	-0.11	0.03
55	1	-0.02	0.03	0.00	0.04	0.01	-0.12	0.13	-0.15	0.03
56	1	-0.02	0.02	-0.03	0.05	0.01	-0.16	0.02	-0.24	0.03
57	1	-0.05	0.01	-0.01	-0.14	0.01	-0.13	0.02	-0.06	0.03
58	1	-0.08	0.00	0.03	-0.09	0.00	-0.20	0.03	-0.18	0.03
59	1	-0.06	0.02	-0.01	-0.09	0.01	-0.15	0.12	-0.11	0.06
60	6	0.00	-0.02	0.00	0.14	0.01	0.05	-0.01	0.06	0.07
61	1	-0.05	-0.05	-0.02	0.12	0.00	0.05	0.01	0.07	0.06
62	1	0.04	-0.05	0.00	0.15	-0.02	0.09	-0.02	0.05	0.11
63	1	0.00	0.03	0.02	0.18	0.05	0.05	0.00	0.07	0.08

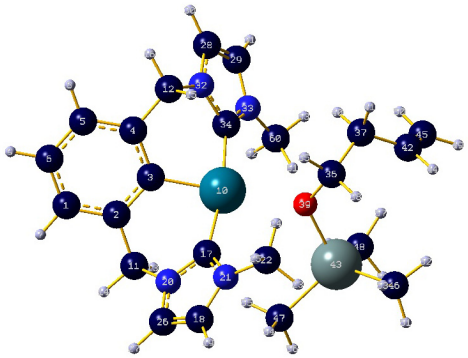
thermodynamics:
Sum of electronic and zero-point Energies= -1319.528927

Sum of electronic and thermal Enthalpies= -1319.493620

Sum of electronic and thermal Free Energies= -1319.596479

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1320.069725

Optimized geometry, SCF energy, three lower frequencies, thermochemistry and PCM energy for **B3.**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.024483	-0.007381	0.001464
2	6	0	-0.017257	-0.002082	1.399509
3	6	0	1.194797	-0.000039	2.107522
4	6	0	2.394184	0.001443	1.378466
5	6	0	2.376473	0.004348	-0.019514
6	6	0	1.169829	-0.002144	-0.712215
7	1	0	-0.972948	-0.008100	-0.532109
8	1	0	3.315374	0.004427	-0.569719
9	1	0	1.160301	-0.003032	-1.798181
10	46	0	1.205839	-0.007273	4.108670
11	6	0	-1.324439	0.052846	2.153122
12	6	0	3.713996	-0.052030	2.109361
13	1	0	-1.497194	-0.862316	2.730751
14	1	0	-2.169869	0.184466	1.473412
15	1	0	3.895654	0.863317	2.683818
16	1	0	4.547763	-0.183583	1.415457
17	6	0	-0.297472	1.382455	3.947161
18	6	0	-1.728034	3.130195	4.000394
19	1	0	-2.105475	4.091504	4.314914

20	7	0	-1.315562	1.187324	3.079102
21	7	0	-0.558000	2.590333	4.507506
22	6	0	0.291132	3.280926	5.460799
23	1	0	-0.199093	3.351670	6.436638
24	1	0	1.223533	2.728537	5.558440
25	1	0	0.510097	4.288630	5.097127
26	6	0	-2.204045	2.240970	3.091989
27	1	0	-3.082134	2.272476	2.464960
28	6	0	4.607727	-2.241907	3.031096
29	6	0	4.156263	-3.122554	3.960606
30	1	0	5.473843	-2.274280	2.387752
31	1	0	4.545604	-4.078040	4.277963
32	7	0	3.721369	-1.186016	3.036081
33	7	0	3.007099	-2.573387	4.501183
34	6	0	2.726942	-1.375044	3.932161
35	1	0	2.830917	1.229577	6.045256
36	6	0	2.396978	0.694124	6.898420
37	6	0	3.489575	-0.182342	7.514744
38	1	0	2.081256	1.452056	7.631376
39	8	0	1.254279	-0.015299	6.407037
40	1	0	3.729387	-1.003400	6.829853
41	1	0	4.389494	0.451455	7.568905
42	6	0	3.201805	-0.699781	8.893393
43	50	0	-0.337084	-0.435691	7.603491
44	1	0	2.911078	0.052693	9.629649
45	6	0	3.342032	-1.965578	9.291815
46	6	0	-0.270141	1.006309	9.186214
47	6	0	-2.061009	-0.216105	6.358532
48	6	0	-0.209649	-2.467750	8.261512
49	1	0	3.168639	-2.263867	10.322362
50	1	0	3.666334	-2.748238	8.608164
51	1	0	-1.239153	1.003267	9.697292
52	1	0	0.501541	0.766549	9.921974
53	1	0	-0.094407	2.017653	8.807604
54	1	0	-2.251963	0.825534	6.089365
55	1	0	-1.951121	-0.803898	5.442859
56	1	0	-2.930618	-0.598031	6.905431
57	1	0	0.781796	-2.690660	8.661237
58	1	0	-0.946805	-2.618648	9.058311
59	1	0	-0.447333	-3.160803	7.449018
60	6	0	2.154417	-3.254038	5.459579
61	1	0	1.606901	-2.503905	6.027476
62	1	0	1.453767	-3.918298	4.944182
63	1	0	2.771024	-3.843225	6.142263

HF=-1320.1121591

	1			2			3		
	A			A			A		
Frequencies --	24.1840			33.3584			38.0190		
Red. masses --	4.8306			4.1634			3.9756		
Frc consts --	0.0017			0.0027			0.0034		
IR Inten --	0.3974			0.1937			0.1613		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	0.10	0.05	-0.04	0.04	0.09	-0.04	0.01	0.05	0.00
2 6	0.06	0.01	-0.04	0.02	0.04	-0.04	0.00	0.04	0.00
3 6	0.04	0.01	0.00	0.01	0.01	-0.02	0.00	0.01	0.00
4 6	0.06	0.03	0.04	0.02	0.03	0.00	0.00	-0.02	0.01
5 6	0.10	0.06	0.04	0.04	0.08	0.00	0.01	-0.01	0.01
6 6	0.13	0.07	0.00	0.05	0.11	-0.02	0.01	0.03	0.00
7 1	0.12	0.05	-0.07	0.05	0.11	-0.06	0.01	0.08	0.00
8 1	0.12	0.08	0.07	0.05	0.10	0.01	0.01	-0.04	0.01
9 1	0.16	0.10	0.00	0.07	0.15	-0.02	0.01	0.03	0.00
10 46	-0.02	-0.01	0.00	-0.02	-0.02	-0.02	-0.01	0.01	0.00
11 6	0.04	-0.02	-0.08	0.01	0.01	-0.06	0.00	0.07	-0.01
12 6	0.04	0.01	0.08	0.01	0.00	0.01	0.00	-0.06	0.01
13 1	0.04	-0.03	-0.09	0.01	-0.01	-0.08	-0.02	0.07	-0.01
14 1	0.05	-0.03	-0.10	0.02	0.02	-0.07	0.01	0.08	-0.01
15 1	0.02	0.00	0.11	0.02	-0.02	0.04	0.03	-0.06	0.00

```
  16   1     0.06   0.02   0.10     0.02   0.00   0.02     0.00  -0.08   0.01
  17   6    -0.04  -0.02  -0.03    -0.02  -0.02  -0.01     0.02   0.04   0.01
  18   6    -0.08  -0.06  -0.05    -0.04  -0.04   0.01     0.03   0.06   0.02
  19   1    -0.11  -0.07  -0.04    -0.05  -0.05   0.03     0.04   0.06   0.02
  20   7    -0.01  -0.03  -0.06    -0.01  -0.01  -0.03     0.02   0.06   0.00
  21   7    -0.09  -0.04  -0.02    -0.04  -0.04   0.01     0.02   0.04   0.02
  22   6    -0.13  -0.03   0.02    -0.05  -0.05   0.03     0.03   0.03   0.02
  23   1    -0.17  -0.04   0.00    -0.06  -0.07   0.03     0.04   0.00   0.03
  24   1    -0.13  -0.02   0.05    -0.05  -0.05   0.03     0.04   0.04   0.00
  25   1    -0.13  -0.02   0.03    -0.05  -0.04   0.05     0.01   0.04   0.04
  26   6    -0.04  -0.05  -0.07    -0.02  -0.02  -0.01     0.03   0.07   0.01
  27   1    -0.02  -0.07  -0.10    -0.01  -0.02  -0.02     0.03   0.08   0.00
  28   6    -0.03  -0.03   0.05    -0.03  -0.03  -0.03    -0.06  -0.08   0.02
  29   6    -0.07  -0.05   0.01    -0.05  -0.05  -0.05    -0.08  -0.05   0.03
  30   1    -0.01  -0.03   0.08    -0.02  -0.03  -0.02    -0.06  -0.10   0.02
  31   1    -0.11  -0.07   0.00    -0.06  -0.06  -0.06    -0.10  -0.06   0.04
  32   7     0.00  -0.01   0.06    -0.01  -0.02  -0.01    -0.03  -0.06   0.01
  33   7    -0.08  -0.04  -0.01    -0.04  -0.04  -0.05    -0.06  -0.02   0.03
  34   6    -0.03  -0.01   0.02    -0.02  -0.03  -0.03    -0.04  -0.02   0.01
  35   1    -0.05   0.05  -0.02     0.06  -0.11  -0.09    -0.05   0.06   0.00
  36   6    -0.01   0.01  -0.02     0.03  -0.03  -0.06    -0.03   0.05   0.00
  37   6     0.03   0.00  -0.11    -0.01  -0.04   0.02     0.01   0.10   0.00
  38   1     0.02  -0.02   0.02     0.05   0.03  -0.11    -0.07   0.04  -0.01
  39   8    -0.02   0.02   0.00     0.01  -0.02  -0.02     0.00  -0.01   0.00
  40   1     0.02   0.04  -0.16    -0.09  -0.14   0.11     0.06   0.11   0.00
  41   1     0.02   0.02  -0.11     0.04  -0.10  -0.08    -0.02   0.15   0.00
  42   6     0.09  -0.07  -0.12    -0.01   0.15   0.09     0.05   0.09   0.00
  43  50     0.01   0.03   0.04     0.04   0.00   0.03     0.00  -0.05  -0.02
  44   1     0.07  -0.12  -0.08     0.10   0.28   0.02    -0.02   0.08   0.00
  45   6     0.16  -0.09  -0.19    -0.15   0.18   0.23     0.15   0.11   0.01
  46   6     0.05   0.04   0.03     0.07   0.01   0.01    -0.11   0.03  -0.08
  47   6    -0.01   0.02   0.06     0.02   0.00   0.05     0.03  -0.22  -0.10
  48   6     0.03   0.04   0.07     0.02   0.00   0.03     0.11   0.01   0.12
  49   1     0.20  -0.14  -0.20    -0.15   0.32   0.27     0.17   0.10   0.02
  50   1     0.18  -0.04  -0.23    -0.28   0.07   0.31     0.22   0.13   0.02
  51   1     0.07   0.04   0.06     0.07   0.05   0.01    -0.11  -0.01  -0.09
  52   1     0.08   0.05   0.00     0.07   0.00   0.01    -0.09   0.10  -0.07
  53   1     0.03   0.04   0.01     0.10   0.00  -0.01    -0.16   0.02  -0.12
  54   1    -0.02   0.02   0.07     0.01   0.00   0.06    -0.06  -0.24  -0.10
  55   1    -0.01   0.03   0.06     0.02   0.01   0.04     0.14  -0.20  -0.10
  56   1     0.00   0.00   0.06     0.03  -0.01   0.05     0.05  -0.32  -0.14
  57   1     0.06   0.04   0.00     0.01  -0.01   0.03     0.14   0.08   0.09
  58   1     0.09   0.07   0.14     0.02   0.00   0.03     0.16   0.04   0.17
  59   1    -0.04   0.03   0.11     0.01   0.00   0.03     0.10  -0.07   0.19
  60   6    -0.12  -0.04  -0.05    -0.06  -0.05  -0.06    -0.07   0.01   0.04
  61   1    -0.11  -0.04  -0.04    -0.07  -0.05  -0.07    -0.03   0.03   0.05
  62   1    -0.13   0.00  -0.09    -0.05  -0.05  -0.08    -0.11   0.04   0.06
  63   1    -0.16  -0.08  -0.05    -0.06  -0.05  -0.06    -0.08  -0.01   0.03

thermodynamics:
Sum of electronic and zero-point Energies=          -1319.584847

Sum of electronic and thermal Enthalpies=           -1319.549486

Sum of electronic and thermal Free Energies=        -1319.651612

  Total free energy in solution:
  with all non electrostatic terms            (a.u.) =   -1320.129775
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V. Reference 48

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