Electronic Supplementary Information

Formation of *S*-alkyl thiophenium ionic liquids: mechanistic rationale and structural relationships

María A. Schiel,*[a] Juan García de la Concepción,[b] Claudia E. Domini,[a] Pedro Cintas[b] and Gustavo F. Silbestri*[a]

[a]INQUISUR, Departamento de Química, Universidad Nacional del Sur (UNS)-CONICET, Av. Alem 1253, B8000CPB Bahía Blanca, Argentina.

[b]Departamento de Química Orgánica e Inorgánica, Facultad de Ciencias, and IACYS-Unidad de Química Verde y Desarrollo Sostenible, Universidad de Extremadura, Avda. de Elvas s/n, 06006 Badajoz, Spain.

schiel.ayelen@uns.edu.ar (M.A. Schiel); gsilbestri@uns.edu.ar (G.F. Silbestri)

This section contains the coordinates, electronic + zpe, and main vibrational data of all optimized species in their corresponding solvent.

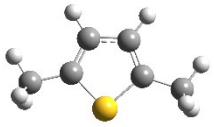
Table of contents

Synthesis

Thiophenes

2,5-dmt (in DCE)

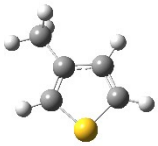
Sum of electronic and zero-point Energies= -631.460670 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.492018 (Hartree/particle)
No imaginary frequencies
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.259461	-0.126192	0.000022
2	6	0	0.715997	-1.374896	-0.000084
3	6	0	-0.715998	-1.374896	0.000070
4	6	0	-1.259461	-0.126192	-0.000005
5	16	0	0.000000	1.075301	-0.000014
6	1	0	1.322802	-2.273286	-0.000135
7	1	0	-1.322802	-2.273286	0.000108
8	6	0	-2.703028	0.265751	-0.000003
9	1	0	-2.962525	0.857031	0.881860
10	1	0	-2.962554	0.856984	-0.881890
11	1	0	-3.325006	-0.631109	0.000033
12	6	0	2.703028	0.265751	0.000029
13	1	0	2.962532	0.857024	-0.881837
14	1	0	2.962547	0.856990	0.881913
15	1	0	3.325006	-0.631109	0.000004

3-mt (in DCE)

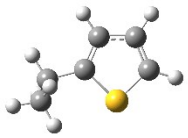
Sum of electronic and zero-point Energies= -592.181787 (Hartree/particle)
Sum of electronic and thermal Free Energies= -592.211719 (Hartree/particle)
No imaginary frequencies
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035859	1.147027	-0.000173
2	6	0	-0.321363	1.244860	0.000149
3	6	0	-0.979783	-0.030217	-0.000073
4	6	0	-0.080638	-1.056151	-0.000053
5	16	0	1.553616	-0.497477	0.000060
6	1	0	-0.850927	2.190530	0.000269
7	1	0	-0.285431	-2.118020	-0.000053
8	1	0	1.766255	1.943874	-0.000259
9	6	0	-2.470958	-0.197061	-0.000009
10	1	0	-2.918363	0.271955	0.880282
11	1	0	-2.918494	0.272381	-0.880004
12	1	0	-2.749603	-1.251831	-0.000234

2-et (in DCE)

Sum of electronic and zero-point Energies= -631.456379 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.488304 (Hartree/particle)
No imaginary frequencies

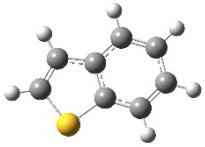


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.016478	-0.441585	0.170571
2	6	0	1.926122	0.914625	0.227529
3	6	0	0.594579	1.384632	-0.001597
4	6	0	-0.305263	0.383956	-0.228731
5	16	0	0.483715	-1.163512	-0.160734
6	1	0	2.772149	1.560189	0.427914
7	1	0	0.312507	2.431277	0.000292
8	6	0	-1.777767	0.497181	-0.494808
9	1	0	-2.008757	0.093604	-1.485801
10	1	0	-2.024010	1.561858	-0.524574
11	6	0	-2.637869	-0.206874	0.556458
12	1	0	-3.699098	-0.049642	0.351309
13	1	0	-2.456823	-1.284647	0.562980
14	1	0	-2.421916	0.176968	1.556349
15	1	0	2.888822	-1.065028	0.306740

bt (in DCE)

Sum of electronic and zero-point Energies= -706.481805 (Hartree/particle)
Sum of electronic and thermal Free Energies= -706.512792 (Hartree/particle)
No imaginary frequencies
Standard orientation:



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

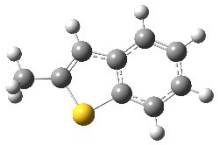
1	6	0	0.109426	0.847375	0.000063
2	6	0	-0.062143	-0.551281	-0.000037
3	6	0	1.028414	-1.425475	0.000061
4	6	0	2.302171	-0.882225	0.000255
5	6	0	2.493040	0.510354	0.000355
6	6	0	1.411912	1.372676	0.000260
7	6	0	-1.152763	1.545399	-0.000067
8	6	0	-2.211104	0.705094	-0.000253
9	1	0	0.880986	-2.499791	-0.000016
10	1	0	3.163103	-1.541422	0.000332
11	1	0	3.500960	0.909877	0.000510
12	1	0	1.560387	2.447496	0.000335
13	1	0	-1.242039	2.624635	-0.000021
14	1	0	-3.261330	0.963140	-0.000374
15	16	0	-1.757236	-0.977215	-0.000286

2-mbt (in DCE)

Sum of electronic and zero-point Energies= -745.762621 (Hartree/particle)
Sum of electronic and thermal Free Energies= -745.796033 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.399704	0.792853	-0.000101
2	6	0	-0.427481	-0.615580	-0.000053
3	6	0	-1.628615	-1.327121	-0.000167
4	6	0	-2.815826	-0.610946	-0.000318
5	6	0	-2.808461	0.793174	-0.000361
6	6	0	-1.614902	1.494708	-0.000257
7	6	0	0.948531	1.305382	0.000047
8	6	0	1.895966	0.338631	0.000216
9	1	0	-1.634627	-2.411612	-0.000132
10	1	0	-3.760074	-1.143956	-0.000406
11	1	0	-3.749306	1.332280	-0.000478
12	1	0	-1.610726	2.579824	-0.000289
13	1	0	1.187134	2.362975	0.000041
14	16	0	1.192259	-1.270802	0.000183
15	6	0	3.381845	0.494853	0.000453
16	1	0	3.830796	0.031793	0.882630
17	1	0	3.831151	0.031379	-0.881323
18	1	0	3.641395	1.554434	0.000266



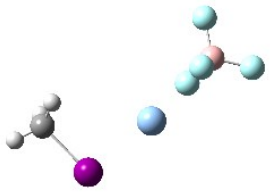
Alkylating intermediates

BF_4-Ag-I-CH_3

Sum of electronic and zero-point Energies= -621.378978 (Hartree/particle)
Sum of electronic and thermal Free Energies= -621.422031 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.690090	1.899656	-0.000255



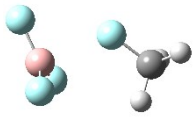
2	1	0	-3.756008	2.100411	0.000874
3	1	0	-2.210571	2.267701	-0.900310
4	1	0	-2.208341	2.268365	0.898368
5	53	0	-2.474029	-0.248568	0.000358
6	47	0	0.371215	-0.229440	-0.000680
7	9	0	2.544082	0.072836	-1.135696
8	5	0	3.399931	0.147696	0.000446
9	9	0	2.543967	0.079950	1.136814
10	9	0	4.272141	-0.931891	0.003694
11	9	0	4.083391	1.355203	-0.003329

F_3B-F-CH_3 (in DCE)

Sum of electronic and zero-point Energies= -464.247239 (Hartree/particle)
Sum of electronic and thermal Free Energies= -464.279890 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.897634	-0.124929	-0.012755
2	6	0	2.205412	-0.133165	-0.000368
3	1	0	2.403298	-0.343591	-1.048941
4	1	0	3.042668	0.378248	0.468155
5	1	0	1.942534	-1.038012	0.544428
6	9	0	-0.862162	-0.538096	1.241555
7	9	0	1.098223	0.741543	0.057000
8	9	0	-0.568729	-0.965320	-0.979408
9	9	0	-1.459865	1.031539	-0.307775

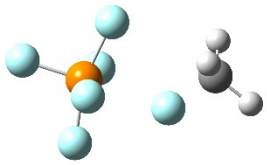


F_5P-F-CH_3 (in DCE)

Sum of electronic and zero-point Energies= -980.355054 (Hartree/particle)
Sum of electronic and thermal Free Energies= -980.389965 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.545391	0.031943	0.000097
2	9	0	-2.030844	0.499694	0.003462
3	9	0	0.146605	1.451167	-0.177990
4	9	0	-0.383806	-0.199770	-1.560887
5	9	0	1.489917	-0.656395	0.000395
6	9	0	-0.782667	-1.523742	0.177223
7	9	0	-0.271069	0.138132	1.559477
8	6	0	2.656129	0.180707	-0.001919
9	1	0	2.627315	0.765078	-0.916341
10	1	0	3.496630	-0.505927	0.019431
11	1	0	2.606917	0.795684	0.891846

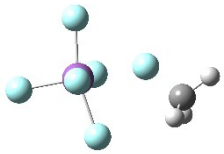


F_5Sb-F-CH_3 (in DCE)

Sum of electronic and zero-point Energies= -644.355819 (Hartree/particle)
Sum of electronic and thermal Free Energies= -644.391634 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	2.125088	-0.630449	0.002696
2	9	0	-0.495336	-1.695950	0.002773
3	9	0	0.136715	0.040264	-1.864613
4	9	0	-1.659585	0.673081	-0.002109
5	9	0	0.708344	1.823081	-0.003530
6	9	0	0.134658	0.047894	1.864121
7	6	0	-2.915596	-0.096740	0.000433
8	1	0	-2.897193	-0.688893	-0.907504
9	1	0	-3.679168	0.672956	-0.000633
10	1	0	-2.895688	-0.685112	0.910777
11	51	0	0.361111	-0.020388	0.000014

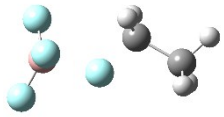


F_3B-F-CH_2CH_3 (in DCE)

Sum of electronic and zero-point Energies= -503.529495 (Hartree/particle)
Sum of electronic and thermal Free Energies= -503.564168 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.572460	0.505422	-0.032670
2	1	0	1.293713	0.977866	0.906725
3	1	0	1.527080	1.207499	-0.861047
4	9	0	-1.133064	0.032558	1.384616
5	9	0	-1.219865	1.203460	-0.579351
6	9	0	-1.788171	-1.022901	-0.543875
7	9	0	0.478159	-0.441446	-0.305179
8	5	0	-1.152841	0.007303	0.037733
9	6	0	2.832731	-0.294657	0.032967
10	1	0	3.658145	0.393972	0.230180
11	1	0	2.793477	-1.025394	0.841396
12	1	0	3.027107	-0.800094	-0.913609

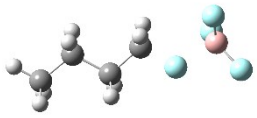


F_3B-F-$CH_2CH_2CH_2CH_3$ (in DCE)

Sum of electronic and zero-point Energies= -582.077281 (Hartree/particle)
Sum of electronic and thermal Free Energies= -582.116612 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.524752	0.420989	-0.189527
2	1	0	0.305388	0.944916	0.739533
3	1	0	0.464624	1.089013	-1.045836
4	9	0	-2.076753	0.033126	1.424510
5	9	0	-2.254950	1.208732	-0.529763
6	9	0	-2.907209	-0.993279	-0.451844
7	9	0	-0.605702	-0.500811	-0.370793
8	5	0	-2.193084	0.009929	0.082728
9	6	0	1.775538	-0.403779	-0.140901
10	1	0	1.707037	-1.119000	0.683778

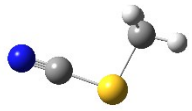


11	1	0	1.875668	-0.966871	-1.073296
12	6	0	2.988306	0.509641	0.054827
13	1	0	2.865767	1.084037	0.978745
14	1	0	3.036558	1.234724	-0.764044
15	6	0	4.286425	-0.287588	0.114030
16	1	0	5.145935	0.369616	0.262631
17	1	0	4.268232	-1.006315	0.937704
18	1	0	4.447610	-0.845255	-0.812414

$NCS\text{-}CH_3$ (in DCE)

Sum of electronic and zero-point Energies= -530.860466 (Hartree/particle)
Sum of electronic and thermal Free Energies= -530.888550 (Hartree/particle)
No imaginary frequencies

Standard orientation:



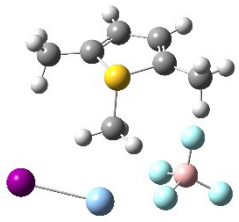
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.465485	0.823704	0.000025
2	1	0	1.262975	1.401471	0.898477
3	1	0	1.262242	1.401786	-0.898053
4	1	0	2.502747	0.491305	-0.000632
5	16	0	0.470767	-0.709464	0.000032
6	6	0	-1.071067	-0.004129	-0.000161
7	7	0	-2.132392	0.448487	0.000074

Thiophenium salts

1,2,5-tmt BF_4 . AgI (in DCE)

Sum of electronic and zero-point Energies= -1252.841667 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1252.896029 (Hartree/particle)
No imaginary frequencies

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.732268	-0.780861	0.202287
2	6	0	-3.852173	-1.168831	-1.073927
3	6	0	-2.913904	-2.201814	-1.503813
4	6	0	-2.061286	-2.629110	-0.563285
5	16	0	-2.459985	-1.784900	0.968169
6	1	0	-4.584057	-0.729844	-1.741738
7	1	0	-2.890617	-2.585533	-2.516917
8	6	0	-1.066876	-0.622097	1.115240
9	1	0	-0.206824	-1.206075	1.441878
10	1	0	-0.911777	-0.166112	0.138891
11	1	0	-1.339105	0.111238	1.872861
12	6	0	-4.466032	0.219426	1.022028
13	1	0	-3.780286	0.928063	1.491448
14	1	0	-5.138916	0.780250	0.372503
15	1	0	-5.053398	-0.265813	1.805274
16	6	0	-0.942495	-3.608891	-0.586926
17	1	0	-0.846549	-4.010742	-1.596154
18	1	0	0.005426	-3.134397	-0.315390

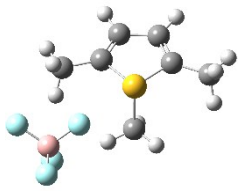
19	1	0	-1.119683	-4.435952	0.104317
20	53	0	2.902410	-1.180019	0.047011
21	47	0	1.524580	1.251580	-0.003547
22	9	0	-0.288815	2.356121	-1.323409
23	5	0	-1.148963	2.741284	-0.261354
24	9	0	-0.432078	2.492117	0.942437
25	9	0	-1.458025	4.089971	-0.360061
26	9	0	-2.299130	1.954754	-0.285125

1,2,5-tmt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1095.739146 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1095.783723 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.910721	-0.450690	-0.185946
2	6	0	-3.347975	0.798920	0.019227
3	6	0	-2.299420	1.808105	0.127657
4	6	0	-1.046053	1.349341	0.004555
5	16	0	-1.129907	-0.404757	-0.362663
6	1	0	-4.401432	1.035225	0.113460
7	1	0	-2.510556	2.854734	0.313553
8	6	0	-0.576329	-1.155765	1.197020
9	1	0	0.485575	-0.934587	1.287939
10	1	0	-1.156815	-0.728747	2.012459
11	1	0	-0.733004	-2.229643	1.106262
12	6	0	-3.628024	-1.747262	-0.323452
13	1	0	-3.277123	-2.474477	0.414008
14	1	0	-4.694092	-1.583146	-0.163155
15	1	0	-3.486536	-2.179556	-1.316698
16	6	0	0.271400	2.034134	0.081654
17	1	0	0.101333	3.085177	0.319014
18	1	0	0.902247	1.597202	0.859756
19	1	0	0.811842	1.965286	-0.863218
20	9	0	3.345405	1.024830	-0.476422
21	9	0	2.607135	-0.243970	1.288923
22	9	0	3.816171	-1.220504	-0.402187
23	9	0	1.664740	-0.512903	-0.780337
24	5	0	2.871748	-0.235828	-0.094973

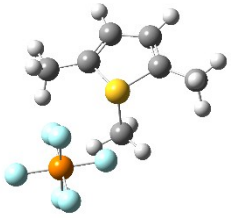


1,2,5-tmt PF_6 (in DCE)

Sum of electronic and zero-point Energies= -1611.862309 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1611.908624 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.486296	-0.477425	-0.190664
2	6	0	-3.951226	0.763381	0.006947
3	6	0	-2.924942	1.794742	0.119704
4	6	0	-1.661327	1.362032	0.007513
5	16	0	-1.705562	-0.394638	-0.354279



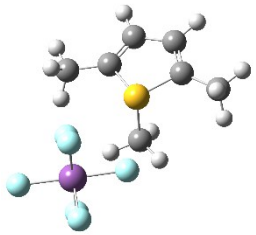
6	1	0	-5.010092	0.977792	0.092524
7	1	0	-3.159403	2.837305	0.300420
8	6	0	-1.148067	-1.128713	1.212056
9	1	0	-0.091756	-0.884958	1.310114
10	1	0	-1.743503	-0.711319	2.021678
11	1	0	-1.281468	-2.205941	1.123831
12	6	0	-4.175157	-1.789238	-0.329041
13	1	0	-3.814611	-2.506488	0.413509
14	1	0	-5.245611	-1.647049	-0.177248
15	1	0	-4.017163	-2.221722	-1.319713
16	6	0	-0.359163	2.074625	0.092058
17	1	0	-0.553044	3.122633	0.324527
18	1	0	0.274858	1.653612	0.876333
19	1	0	0.189690	2.014052	-0.848523
20	9	0	1.480711	1.067922	0.071323
21	9	0	1.375086	-0.847672	0.834569
22	9	0	3.098371	-1.349371	-0.186117
23	9	0	1.488804	-0.554252	-1.206058
24	9	0	3.203986	0.566222	-0.949367
25	9	0	3.090273	0.272793	1.091265
26	15	0	2.289539	-0.140726	-0.057398

1,2,5-tmt SbF_6 (in DCE)

Sum of electronic and zero-point Energies= -1275.867197 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1275.917076 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.538787	-1.116613	-0.217389
2	6	0	-4.589063	-0.297233	-0.363437
3	6	0	-4.273050	1.126852	-0.302997
4	6	0	-2.978126	1.415991	-0.111283
5	16	0	-2.058038	-0.119811	-0.104562
6	1	0	-5.597865	-0.669085	-0.499246
7	1	0	-5.028624	1.898824	-0.391767
8	6	0	-1.616609	-0.296131	1.649511
9	1	0	-0.883893	0.478380	1.867676
10	1	0	-2.519365	-0.178671	2.245717
11	1	0	-1.170927	-1.281677	1.767998
12	6	0	-3.423684	-2.599703	-0.184186
13	1	0	-3.008328	-2.942924	0.767661
14	1	0	-4.415212	-3.037723	-0.303821
15	1	0	-2.779402	-2.968860	-0.985367
16	6	0	-2.255665	2.707561	0.035656
17	1	0	-2.981386	3.521131	0.001394
18	1	0	-1.723676	2.757636	0.989249
19	1	0	-1.526283	2.850430	-0.763605
20	9	0	0.472268	1.195773	-0.032483
21	9	0	1.947071	-0.003518	1.838495
22	9	0	3.324373	-1.316429	-0.073625
23	9	0	0.631802	-1.436830	0.010590
24	9	0	1.843621	-0.065562	-1.956660
25	9	0	3.164559	1.391480	-0.111900
26	51	0	1.924710	-0.039981	-0.061331

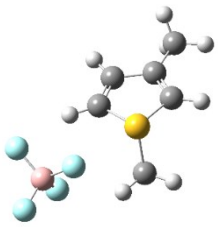


1,3-dmt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1056.456481 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1056.498774 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.589139	-0.841171	-0.307616
2	6	0	-2.994948	0.392248	0.028013
3	6	0	-1.876500	1.342595	0.129471
4	6	0	-0.673303	0.822661	-0.123915
5	16	0	-0.847367	-0.874616	-0.611395
6	1	0	-2.025428	2.383233	0.393865
7	6	0	-0.238504	-1.829803	0.815855
8	1	0	0.844704	-1.841743	0.745203
9	1	0	-0.586701	-1.348892	1.727248
10	1	0	-0.649291	-2.832362	0.705414
11	9	0	2.592391	1.630952	-0.324609
12	9	0	2.169397	0.087631	1.314422
13	9	0	4.022376	-0.145495	-0.027827
14	9	0	1.916783	-0.485016	-0.885752
15	5	0	2.694787	0.275499	0.023487
16	1	0	0.303104	1.283030	-0.153096
17	1	0	-3.163674	-1.743105	-0.466650
18	6	0	-4.404602	0.804914	0.285912
19	1	0	-4.493362	1.229325	1.289128
20	1	0	-4.701549	1.581985	-0.423117
21	1	0	-5.090417	-0.036412	0.194466

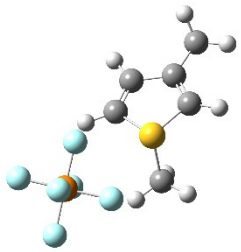


1,3-dmt PF_6 (in DCE)

Sum of electronic and zero-point Energies= -1572.577806 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1572.622495 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.155458	-0.741457	-0.623253
2	6	0	-3.782335	0.336811	-0.128932
3	6	0	-2.864847	1.252441	0.568179
4	6	0	-1.588991	0.860433	0.582481
5	16	0	-1.410850	-0.631149	-0.359755
6	1	0	-3.208186	2.167514	1.036802
7	6	0	-1.115976	-1.898625	0.914273
8	1	0	-0.108583	-1.737765	1.288664
9	1	0	-1.867241	-1.787707	1.693128
10	1	0	-1.189166	-2.862324	0.413194
11	9	0	2.954090	1.520590	0.466214
12	9	0	1.320815	0.104940	1.261115
13	9	0	3.207224	0.179533	-1.389623
14	9	0	1.130524	1.005687	-0.834357
15	15	0	2.281586	0.146304	-0.063901
16	1	0	-0.705485	1.319007	1.000388
17	1	0	-3.545691	-1.577631	-1.186775
18	6	0	-5.243693	0.615458	-0.238216
19	1	0	-5.676802	0.737849	0.757842
20	1	0	-5.406769	1.550068	-0.780897



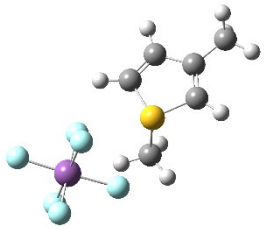
21	1	0	-5.764294	-0.189201	-0.756021
22	9	0	3.402611	-0.719451	0.720348
23	9	0	1.576938	-1.232007	-0.579133

1,3-dmt SbF_6 (in DCE)

Sum of electronic and zero-point Energies= -1236.544097 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1236.631132 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.910523	0.222772	0.748468
2	6	0	-3.190065	1.166693	0.075988
3	6	0	-2.653280	0.643148	-1.148770
4	6	0	-2.981398	-0.659193	-1.365489
5	16	0	-3.954902	-1.289256	-0.088691
6	1	0	-2.041832	1.225537	-1.828192
7	6	0	-0.791981	-1.468078	1.149288
8	1	0	-0.768374	-2.243698	0.392128
9	1	0	-1.329828	-0.572557	0.857034
10	1	0	-1.051026	-1.828907	2.138205
11	9	0	2.871185	0.315235	1.442251
12	9	0	0.451507	-0.455954	-1.275188
13	9	0	0.613187	-1.033124	1.300660
14	9	0	2.629266	-1.599252	-0.352168
15	9	0	2.851660	1.043238	-1.287053
16	9	0	0.702795	1.484837	0.469733
17	1	0	-4.427255	0.329923	1.692608
18	1	0	-2.705519	-1.291699	-2.197711
19	6	0	-2.967335	2.575430	0.541428
20	1	0	-3.443488	2.753141	1.506623
21	1	0	-1.899656	2.786497	0.642119
22	1	0	-3.374104	3.291654	-0.177274
23	51	0	1.808051	0.068603	-0.084237

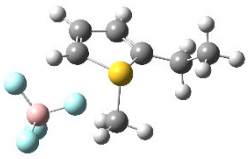


2e1-mt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1095.730977 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1095.775234 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.448367	0.370415	0.153342
2	6	0	-2.369138	1.706023	0.228062
3	6	0	-1.032486	2.250204	0.004142
4	6	0	-0.090262	1.329448	-0.226624
5	16	0	-0.832636	-0.276268	-0.294518
6	1	0	-3.227803	2.326307	0.455913
7	1	0	-0.817687	3.311457	0.025148
8	6	0	-0.371741	-1.087628	1.268394
9	1	0	0.648808	-1.437727	1.152475
10	1	0	-0.471063	-0.365169	2.075731
11	1	0	-1.059198	-1.924842	1.385892
12	6	0	-3.588029	-0.570962	0.359151



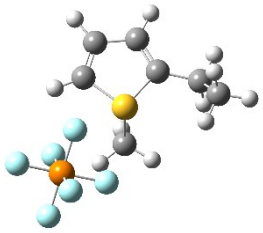
13	1	0	-3.379646	-1.203149	1.230097
14	1	0	-4.458695	0.037907	0.613392
15	9	0	3.206857	1.005180	-0.759513
16	9	0	2.500414	0.085764	1.216032
17	9	0	4.070987	-1.007820	-0.058875
18	9	0	1.888319	-0.869155	-0.770572
19	5	0	2.936235	-0.198350	-0.090221
20	1	0	0.958542	1.437811	-0.458892
21	6	0	-3.879264	-1.444921	-0.861786
22	1	0	-3.045095	-2.113954	-1.089290
23	1	0	-4.756759	-2.065698	-0.674449
24	1	0	-4.073890	-0.832110	-1.744347

2e1-mt PF_6 (in DCE)

Sum of electronic and zero-point Energies= -1611.853062 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1611.900123 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.124662	0.079409	-0.080879
2	6	0	-3.510989	1.322447	-0.401192
3	6	0	-2.437308	2.313148	-0.405653
4	6	0	-1.234961	1.825197	-0.079784
5	16	0	-1.341957	0.071942	0.123536
6	1	0	-4.542778	1.571279	-0.619358
7	1	0	-2.601230	3.356027	-0.647427
8	6	0	-1.187104	-0.206831	1.914596
9	1	0	-0.155722	0.015181	2.175328
10	1	0	-1.889098	0.443261	2.432607
11	1	0	-1.403710	-1.261168	2.084119
12	6	0	-3.890773	-1.189459	0.093379
13	1	0	-3.860804	-1.481011	1.149507
14	1	0	-4.933794	-0.964023	-0.141542
15	9	0	1.425715	0.178754	-1.389553
16	9	0	1.461434	0.904750	0.784277
17	9	0	3.306609	-0.408725	1.192140
18	9	0	1.390961	-1.340074	0.333978
19	1	0	-0.266000	2.297672	-0.024502
20	6	0	-3.375000	-2.335743	-0.777485
21	1	0	-2.357142	-2.626725	-0.503102
22	1	0	-4.010894	-3.213508	-0.653221
23	1	0	-3.374911	-2.057279	-1.833289
24	9	0	3.267963	-1.143308	-0.990263
25	9	0	3.340495	1.112320	-0.529017
26	15	0	2.379573	-0.120882	-0.105843



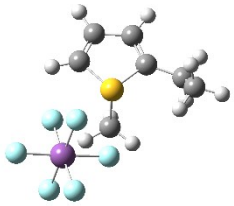
2e1-mt SbF_6 (in DCE)

Sum of electronic and zero-point Energies= -1275.858472 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1275.908692 (Hartree/particle)
No imaginary frequencies

Standard orientation:

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

1	6	0	3.694273	0.166297	-0.047246
2	6	0	4.388340	-0.933740	-0.372044
3	6	0	3.586217	-2.151129	-0.478062
4	6	0	2.282899	-1.974115	-0.233253
5	16	0	1.955196	-0.258578	0.029725
6	1	0	5.460757	-0.921255	-0.525222
7	1	0	4.011880	-3.114675	-0.729753
8	6	0	1.637170	-0.136649	1.816619
9	1	0	0.677247	-0.613251	1.999739
10	1	0	2.446041	-0.636590	2.345617
11	1	0	1.587621	0.925085	2.052571
12	6	0	4.111932	1.575545	0.213196
13	1	0	3.987403	1.789952	1.281148
14	1	0	5.181504	1.636793	-0.000096
15	9	0	-0.610137	-1.307352	0.018535
16	9	0	-2.359602	-0.294025	1.762520
17	9	0	-3.250006	1.426288	-0.115325
18	9	0	-0.614444	1.280493	0.487989
19	9	0	-1.478993	0.360370	-1.868586
20	9	0	-3.233453	-1.246182	-0.598647
21	51	0	-1.956467	0.044920	-0.060111
22	1	0	1.452007	-2.663497	-0.257121
23	6	0	3.332832	2.599002	-0.614154
24	1	0	2.273792	2.618734	-0.340029
25	1	0	3.733238	3.599492	-0.444204
26	1	0	3.402937	2.377956	-1.681306

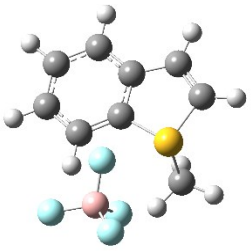


1-mbt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1170.759288 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1170.803481 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.390587	-0.067083	-0.356064
2	6	0	1.067937	-0.139721	0.095197
3	6	0	0.485213	-1.303919	0.560469
4	6	0	1.284938	-2.446727	0.572640
5	6	0	2.603274	-2.406655	0.118876
6	6	0	3.165874	-1.223361	-0.350419
7	6	0	2.776484	1.281846	-0.766728
8	6	0	1.813100	2.193788	-0.621881
9	1	0	-0.541738	-1.333895	0.900209
10	1	0	0.866777	-3.378759	0.934276
11	1	0	3.198375	-3.312529	0.130020
12	1	0	4.190237	-1.193487	-0.703931
13	1	0	3.763602	1.517245	-1.146761
14	1	0	1.814619	3.250345	-0.850325
15	16	0	0.292266	1.459945	-0.052354
16	6	0	0.228615	2.027300	1.675034
17	1	0	1.207389	1.887025	2.128386
18	1	0	-0.542346	1.435147	2.162522
19	1	0	-0.058697	3.077621	1.649857
20	9	0	-2.137859	0.392631	0.798711
21	9	0	-1.914726	-0.349494	-1.357595
22	9	0	-3.969588	0.332669	-0.587672
23	9	0	-3.041843	-1.622143	0.183194
24	5	0	-2.778892	-0.316723	-0.251812

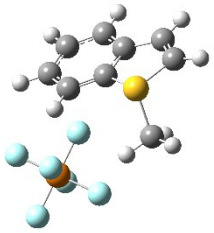


1-mbt PF_6 (in DCE)

Sum of electronic and zero-point Energies= -1686.881335 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1686.927946 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.395596	-0.037103	-0.069417
2	6	0	2.004712	-0.164216	-0.155088
3	6	0	1.341958	-1.375518	-0.086570
4	6	0	2.129549	-2.512469	0.092046
5	6	0	3.518495	-2.417491	0.177959
6	6	0	4.162957	-1.186157	0.095640
7	6	0	3.843090	1.351672	-0.165211
8	6	0	2.855757	2.238739	-0.304395
9	1	0	0.264627	-1.444929	-0.167710
10	1	0	1.649410	-3.481645	0.157735
11	1	0	4.105434	-3.319266	0.309053
12	1	0	5.243027	-1.115977	0.157984
13	1	0	4.888491	1.633711	-0.121502
14	1	0	2.891189	3.314166	-0.407645
15	16	0	1.266384	1.437656	-0.410494
16	6	0	0.539615	1.803719	1.218244
17	1	0	1.320198	1.720710	1.971561
18	1	0	-0.253596	1.076938	1.376614
19	1	0	0.132413	2.812094	1.162302
20	9	0	-1.802853	-0.662489	1.245552
21	9	0	-1.272591	0.333013	-0.752065
22	9	0	-4.036240	-0.634563	0.678567
23	9	0	-2.495452	-1.612579	-0.725799
24	9	0	-3.501741	0.364474	-1.327376
25	9	0	-2.805393	1.311934	0.648216
26	15	0	-2.668352	-0.153563	-0.039572

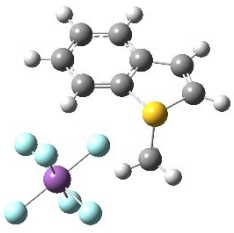


1-mbt SbF_6 (in DCE)

Sum of electronic and zero-point Energies= -1350.886436 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1350.936924 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.018860	0.149584	-0.085543
2	6	0	-2.620655	0.168347	-0.151376
3	6	0	-1.868038	1.324128	-0.061901
4	6	0	-2.567503	2.517189	0.118274
5	6	0	-3.960332	2.530198	0.186811
6	6	0	-4.696412	1.353238	0.082699
7	6	0	-4.572621	-1.198981	-0.197047
8	6	0	-3.654874	-2.158798	-0.327996
9	1	0	-0.788276	1.316413	-0.130826
10	1	0	-2.013677	3.445138	0.198568



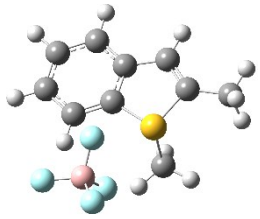
11	1	0	-4.477904	3.473015	0.320906
12	1	0	-5.779343	1.365916	0.130629
13	1	0	-5.637041	-1.399932	-0.169947
14	1	0	-3.776178	-3.227289	-0.439076
15	16	0	-2.005885	-1.486790	-0.407750
16	6	0	-1.341069	-1.927395	1.228447
17	1	0	-2.088438	-1.691982	1.982882
18	1	0	-0.427730	-1.351816	1.361476
19	1	0	-1.117864	-2.993378	1.198959
20	9	0	1.606898	-0.367621	1.707539
21	9	0	0.581946	-0.563266	-0.709362
22	9	0	3.855297	0.753968	0.707187
23	9	0	1.429282	1.788361	0.135426
24	9	0	2.814249	0.506564	-1.784589
25	9	0	2.985753	-1.655802	-0.195933
26	51	0	2.245921	0.081327	-0.027965

1,2-dmbt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1210.043242 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1210.089186 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.179422	0.754164	-0.274074
2	6	0	-0.848219	0.583244	0.122519
3	6	0	-0.010486	1.631208	0.457238
4	6	0	-0.552335	2.914984	0.399518
5	6	0	-1.873994	3.116723	0.002526
6	6	0	-2.695099	2.045586	-0.339014
7	6	0	-2.860168	-0.508404	-0.548477
8	6	0	-2.118371	-1.605938	-0.367638
9	1	0	1.017728	1.469123	0.753883
10	1	0	0.069413	3.763303	0.660206
11	1	0	-2.268305	4.125410	-0.042368
12	1	0	-3.721804	2.207215	-0.647660
13	1	0	-3.897077	-0.555321	-0.862428
14	16	0	-0.433084	-1.148380	0.081889
15	6	0	-0.402889	-1.596986	1.842857
16	1	0	-1.323798	-1.254481	2.310226
17	1	0	0.476276	-1.117119	2.266411
18	1	0	-0.299454	-2.680139	1.892233
19	9	0	2.209540	-0.600104	0.818222
20	9	0	2.093766	0.025612	-1.381707
21	9	0	4.019239	-0.922109	-0.561318
22	9	0	3.416828	1.201364	0.078200
23	5	0	2.948413	-0.072369	-0.272821
24	6	0	-2.444522	-3.051124	-0.503008
25	1	0	-2.334867	-3.570960	0.453152
26	1	0	-3.478428	-3.154408	-0.833610
27	1	0	-1.793744	-3.540307	-1.231431



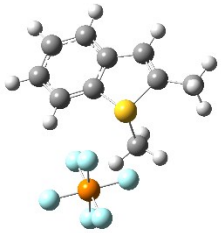
1,2-dmbt PF_6 (in DCE)

Sum of electronic and zero-point Energies= -1726.166388 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1726.214163 (Hartree/particle)

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.291824	0.099713	-0.190802
2	6	0	-1.973214	0.535339	-0.017496
3	6	0	-1.619162	1.863506	0.132801
4	6	0	-2.655806	2.796359	0.123216
5	6	0	-3.979563	2.392667	-0.050110
6	6	0	-4.308967	1.049547	-0.211853
7	6	0	-3.399596	-1.351927	-0.314465
8	6	0	-2.243249	-2.018743	-0.237648
9	1	0	-0.587268	2.168956	0.251747
10	1	0	-2.423054	3.847632	0.244884
11	1	0	-4.766229	3.138644	-0.062109
12	1	0	-5.339180	0.741470	-0.350068
13	1	0	-4.350404	-1.856066	-0.447783
14	16	0	-0.869441	-0.860261	-0.078176
15	6	0	-0.413086	-1.086974	1.666402
16	1	0	-1.322074	-1.092126	2.264445
17	1	0	0.242420	-0.258787	1.926389
18	1	0	0.126303	-2.029853	1.734828
19	9	0	2.135553	-1.228282	0.186085
20	9	0	1.332398	0.921973	0.098809
21	9	0	2.487542	0.050521	-1.686344
22	9	0	3.446655	1.689646	-0.390870
23	6	0	-1.932949	-3.472734	-0.284393
24	1	0	-1.424104	-3.797238	0.627875
25	1	0	-2.863757	-4.032800	-0.377787
26	1	0	-1.290511	-3.716187	-1.133963
27	9	0	3.091671	0.406802	1.481693
28	9	0	4.254028	-0.466010	-0.303337
29	15	0	2.805520	0.229210	-0.106392

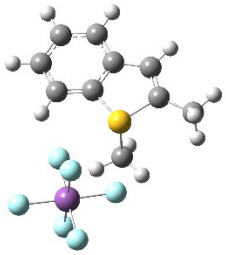


1,2-dmbt SbF_6 (in DCE)

Sum of electronic and zero-point Energies= -1390.171704 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1390.222720 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.918009	0.094304	-0.189305
2	6	0	-2.601348	0.541813	-0.032429
3	6	0	-2.255641	1.873121	0.108285
4	6	0	-3.299768	2.797741	0.103074
5	6	0	-4.622023	2.382608	-0.054300
6	6	0	-4.942714	1.035968	-0.205297
7	6	0	-4.014702	-1.358976	-0.304399
8	6	0	-2.852271	-2.015849	-0.232464
9	1	0	-1.223472	2.183011	0.213919
10	1	0	-3.074352	3.851617	0.215940
11	1	0	-5.414667	3.122274	-0.062310
12	1	0	-5.971880	0.719123	-0.330935
13	1	0	-4.962231	-1.871552	-0.428378
14	16	0	-1.487764	-0.845658	-0.087022



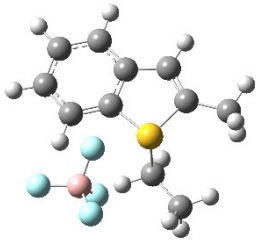
15	6	0	-1.026371	-1.055084	1.658675
16	1	0	-1.934328	-1.061267	2.258328
17	1	0	-0.379548	-0.218297	1.914514
18	1	0	-0.479697	-1.992983	1.734096
19	9	0	1.472808	-1.523062	0.105938
20	9	0	0.648101	0.968557	0.026069
21	9	0	2.193124	0.044565	-1.953818
22	9	0	3.185990	1.850173	-0.216431
23	6	0	-2.529834	-3.467293	-0.275661
24	1	0	-2.006838	-3.782596	0.631768
25	1	0	-3.456475	-4.036366	-0.355125
26	1	0	-1.895111	-3.709001	-1.131553
27	9	0	2.480340	0.251711	1.825024
28	9	0	4.044792	-0.726356	-0.148001
29	51	0	2.367696	0.148356	-0.068118

1e2-mbt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1249.319578 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1249.368545 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.278170	0.842761	-0.234348
2	6	0	-0.928935	0.713358	0.112630
3	6	0	-0.154765	1.764565	0.568690
4	6	0	-0.781398	3.004587	0.690089
5	6	0	-2.123544	3.164752	0.346278
6	6	0	-2.880287	2.092965	-0.118953
7	6	0	-2.875483	-0.416664	-0.668912
8	6	0	-2.054950	-1.472614	-0.652341
9	1	0	0.889473	1.636494	0.821930
10	1	0	-0.209070	3.852917	1.046585
11	1	0	-2.584740	4.141118	0.442664
12	1	0	-3.923000	2.222359	-0.386136
13	1	0	-3.913494	-0.496014	-0.972740
14	16	0	-0.392795	-0.959381	-0.178005
15	6	0	-0.228918	-1.652440	1.528571
16	1	0	-1.235708	-1.671257	1.945935
17	1	0	0.377724	-0.912757	2.048387
18	9	0	2.217644	-0.322282	0.650952
19	9	0	2.027881	0.548591	-1.459199
20	9	0	3.985909	-0.462515	-0.810026
21	9	0	3.385575	1.567432	0.084792
22	5	0	2.916944	0.336137	-0.394186
23	6	0	-2.302569	-2.903553	-0.980363
24	1	0	-2.258360	-3.525385	-0.081951
25	1	0	-3.298800	-3.002041	-1.413424
26	1	0	-1.570651	-3.286804	-1.694825
27	6	0	0.445682	-3.007948	1.476157
28	1	0	0.535915	-3.377714	2.499835
29	1	0	-0.129536	-3.739667	0.907268
30	1	0	1.447193	-2.931487	1.051827



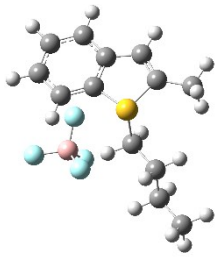
1b2-mbt BF_4 (in DCE)

Sum of electronic and zero-point Energies= -1327.868593 (Hartree/particle)

Sum of electronic and thermal Free Energies= -1327.922062 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.413540	-1.395204	0.036248
2	6	0	1.546580	-0.324613	-0.208635
3	6	0	1.901563	0.793064	-0.941391
4	6	0	3.195049	0.823168	-1.461004
5	6	0	4.084046	-0.226217	-1.227596
6	6	0	3.705660	-1.337827	-0.479217
7	6	0	1.791471	-2.459518	0.819082
8	6	0	0.514209	-2.247688	1.155385
9	1	0	1.209893	1.609094	-1.105385
10	1	0	3.509753	1.680487	-2.044337
11	1	0	5.087686	-0.174108	-1.633883
12	1	0	4.401091	-2.149800	-0.298999
13	1	0	2.321708	-3.362871	1.099783
14	16	0	-0.012686	-0.616538	0.597147
15	6	0	-1.145191	-1.009150	-0.807592
16	1	0	-0.799200	-1.956385	-1.223986
17	1	0	-0.964752	-0.201725	-1.517035
18	9	0	-1.025383	1.847318	-0.284799
19	9	0	0.444421	2.388337	1.387426
20	9	0	-1.625999	3.379218	1.318942
21	9	0	-0.040090	3.916527	-0.254595
22	5	0	-0.562349	2.896158	0.551095
23	6	0	-0.450464	-3.096888	1.906392
24	1	0	-1.263376	-3.436290	1.258552
25	1	0	0.070986	-3.975239	2.288712
26	1	0	-0.891632	-2.556190	2.746822
27	6	0	-2.587638	-1.033562	-0.332351
28	1	0	-2.727919	-1.793362	0.442460
29	1	0	-2.839332	-0.064337	0.106957
30	6	0	-3.518329	-1.326620	-1.509983
31	1	0	-3.249262	-2.289490	-1.956643
32	1	0	-3.368108	-0.566548	-2.283430
33	6	0	-4.981134	-1.344694	-1.080241
34	1	0	-5.637706	-1.556726	-1.927054
35	1	0	-5.159154	-2.110351	-0.319986
36	1	0	-5.278666	-0.380449	-0.659707

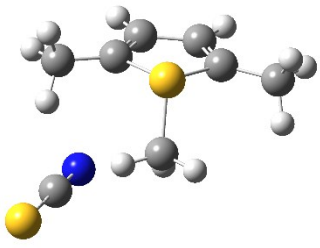


1,2,5-tmt SCN (in DCE)

Sum of electronic and zero-point Energies= -1162.292940 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1162.335418 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.489217	-0.298032	0.277940
2	6	0	-2.406482	0.878163	0.913741
3	6	0	-1.312630	1.744509	0.485639
4	6	0	-0.533207	1.246208	-0.482581
5	16	0	-1.218063	-0.333059	-0.984247
6	1	0	-3.093216	1.152990	1.705762
7	1	0	-1.122642	2.711874	0.935635



8	6	0	-0.025752	-1.530914	-0.313800
9	1	0	0.899858	-1.405965	-0.876406
10	1	0	0.120067	-1.323745	0.743784
11	1	0	-0.443760	-2.521013	-0.490762
12	6	0	-3.402339	-1.462049	0.434559
13	1	0	-3.960196	-1.662411	-0.482883
14	1	0	-2.847742	-2.365948	0.700996
15	1	0	-4.111669	-1.248438	1.234841
16	6	0	0.666801	1.775723	-1.181873
17	1	0	1.012226	2.668495	-0.659245
18	1	0	1.481886	1.046915	-1.186571
19	1	0	0.436280	2.038021	-2.217607
20	16	0	3.701141	-0.666886	-0.140728
21	6	0	2.637296	-0.026832	0.959649
22	7	0	1.870405	0.421098	1.718917

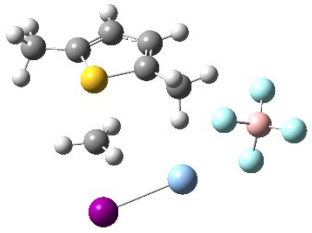
TS- alkylation

TS: BF_4-Ag-I-CH_3 + 2,5-dmt -> 1,2,5-tmt BF_4 . AgI

Sum of electronic and zero-point Energies= -1252.815218 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1252.870430 (Hartree/particle)
1 imaginary frequency (489.8108i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871645	2.254369	-0.852674
2	6	0	1.734764	2.784118	0.382525
3	6	0	2.700148	2.301302	1.343758
4	6	0	3.575549	1.400745	0.845659
5	16	0	3.228231	1.127749	-0.859246
6	1	0	0.957777	3.500693	0.621930
7	1	0	2.725060	2.623382	2.378197
8	6	0	1.903426	-0.739439	-0.532493
9	1	0	2.740266	-1.391739	-0.328733
10	1	0	1.403401	-0.232348	0.279823
11	1	0	1.505325	-0.696684	-1.535342
12	6	0	1.067325	2.466355	-2.090949
13	1	0	0.548091	1.551847	-2.392704
14	1	0	0.316384	3.235548	-1.909521
15	1	0	1.694069	2.785053	-2.926978
16	6	0	4.683263	0.658116	1.514717
17	1	0	4.754496	0.977181	2.555281
18	1	0	4.506054	-0.421040	1.500621
19	1	0	5.644452	0.844558	1.030352
20	53	0	0.227566	-2.804525	-0.074667
21	47	0	-1.620523	-0.690360	0.142508
22	9	0	-3.499183	0.816475	0.573094
23	5	0	-2.929819	2.067622	0.197675
24	9	0	-1.622498	1.771605	-0.275666
25	9	0	-3.682658	2.641957	-0.816833
26	9	0	-2.852452	2.900498	1.306388

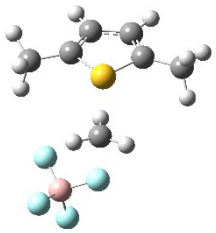


TS: F_3B-F-CH_3 + 2,5- dmt --> 1,2,5-tmt BF_4

Sum of electronic and zero-point Energies= -1095.694052 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1095.740238 (Hartree/particle)
1 imaginary frequency (586.4926i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.629289	0.939749	0.203489
2	6	0	2.751952	0.222182	1.344519
3	6	0	2.252598	-1.127052	1.247212
4	6	0	1.749682	-1.442852	0.031344
5	16	0	1.891066	-0.056749	-1.042767
6	1	0	3.184579	0.637293	2.247370
7	1	0	2.264326	-1.831130	2.070960
8	6	0	-0.416924	0.683728	-0.554021
9	1	0	-0.769445	-0.071990	-1.241505
10	1	0	-0.178952	0.429261	0.469016
11	1	0	-0.182193	1.666462	-0.936363
12	6	0	3.015597	2.352115	-0.088013
13	1	0	2.153795	2.949782	-0.397501
14	1	0	3.437791	2.804146	0.810425
15	1	0	3.762332	2.407768	-0.883737
16	6	0	1.106498	-2.703861	-0.442400
17	1	0	1.152114	-3.452774	0.349539
18	1	0	0.054493	-2.543093	-0.696431
19	1	0	1.606479	-3.105626	-1.326483
20	9	0	-3.462613	-0.380713	-1.077998
21	9	0	-2.451445	-0.805469	0.932307
22	9	0	-4.162798	0.725373	0.809509
23	9	0	-2.116247	1.216752	-0.108956
24	5	0	-3.107323	0.134069	0.154487

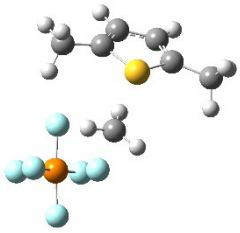


TS: F_5P-F-CH_3 + 2,5- dmt --> 1,2,5-tmt PF_6

Sum of electronic and zero-point Energies= -1611.808132 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1611.855124 (Hartree/particle)
1 imaginary frequency (542.0479i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.297031	0.962029	0.272691
2	6	0	3.178705	0.335800	1.468289
3	6	0	2.700007	-1.019769	1.374791
4	6	0	2.455619	-1.430224	0.107486
5	16	0	2.819490	-0.129464	-1.017209
6	1	0	3.417259	0.825274	2.405306
7	1	0	2.534528	-1.659394	2.233787
8	6	0	0.374726	0.588810	-0.872167
9	1	0	0.128546	-0.336317	-1.374080
10	1	0	0.597198	0.594647	0.184961
11	1	0	0.586288	1.463631	-1.470435
12	6	0	3.733264	2.356214	-0.037670
13	1	0	2.950658	2.914053	-0.559270
14	1	0	3.961920	2.880379	0.891337
15	1	0	4.626640	2.368222	-0.666383
16	6	0	1.919419	-2.731740	-0.390268
17	1	0	1.783653	-3.413410	0.450333
18	1	0	0.950268	-2.603658	-0.882051
19	1	0	2.597817	-3.199475	-1.107440
20	9	0	-3.645167	0.938589	-0.755574
21	9	0	-1.400867	-0.690748	0.873318



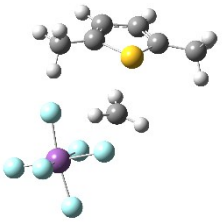
22	9	0	-1.347701	1.073737	-0.635089
23	9	0	-2.397365	-0.923760	-1.153210
24	15	0	-2.584433	0.082785	0.092429
25	9	0	-3.717494	-0.827296	0.753379
26	9	0	-2.650600	1.166030	1.277611

TS: $F_5Sb\text{-}F\text{-}CH_3$ + 2,5- dmt --> 1,2,5-tmt SbF_6

Sum of electronic and zero-point Energies= -1275.813921 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1275.863680 (Hartree/particle)
1 imaginary frequency (521.9417i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.960489	-0.923748	0.288997
2	6	0	-3.765296	-0.320245	1.486040
3	6	0	-3.225288	1.011738	1.389822
4	6	0	-3.011818	1.428280	0.119078
5	16	0	-3.479621	0.160581	-1.005835
6	1	0	-3.990371	-0.810604	2.425925
7	1	0	-2.991305	1.628766	2.249484
8	6	0	-1.058856	-0.637268	-0.926383
9	1	0	-0.805194	0.272007	-1.453446
10	1	0	-1.249611	-0.617340	0.137438
11	1	0	-1.307801	-1.517799	-1.500898
12	6	0	-4.481846	-2.288918	-0.019228
13	1	0	-3.759143	-2.875447	-0.592764
14	1	0	-4.685714	-2.818238	0.912607
15	1	0	-5.407784	-2.245125	-0.597434
16	6	0	-2.433282	2.710859	-0.380072
17	1	0	-2.164235	3.339567	0.469844
18	1	0	-1.531099	2.541550	-0.975434
19	1	0	-3.144384	3.258413	-1.003206
20	9	0	3.312644	-1.303710	-0.704586
21	9	0	0.722512	1.037383	0.711002
22	9	0	0.658231	-1.143194	-0.724201
23	9	0	2.089144	0.917437	-1.557894
24	9	0	3.481531	1.009127	0.804670
25	9	0	1.966444	-1.143549	1.598287
26	51	0	2.122692	-0.058249	0.061298

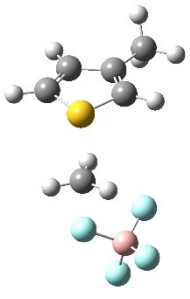


TS: $F_3B\text{-}F\text{-}CH_3$ + 3-mt --> 1,3-dmt BF_4

Sum of electronic and zero-point Energies= -1056.411712 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1056.455653 (Hartree/particle)
1 imaginary frequency (589.4825i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.072252	0.225967	-1.052344
2	6	0	2.627386	0.943673	-0.046266
3	6	0	2.867275	0.128877	1.127497
4	6	0	2.493122	-1.160221	0.977884
5	16	0	1.839667	-1.443098	-0.612084
6	1	0	3.300323	0.521472	2.040030
7	6	0	-0.503251	-1.118898	0.094575

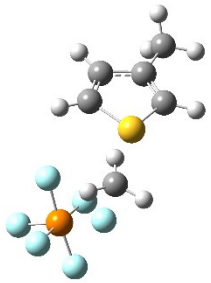


8	1	0	-0.478736	-2.066582	0.611460
9	1	0	-0.136919	-0.226474	0.581664
10	1	0	-0.793161	-1.093724	-0.946177
11	9	0	-4.072648	0.552094	0.803668
12	9	0	-2.085268	1.379108	-0.004174
13	9	0	-3.284695	-0.126654	-1.245059
14	9	0	-2.229253	-0.809946	0.682439
15	5	0	-2.962391	0.307435	0.027838
16	1	0	2.554545	-1.975294	1.685174
17	1	0	1.778024	0.561217	-2.037299
18	6	0	2.955153	2.403444	-0.110553
19	1	0	2.671187	2.829261	-1.073063
20	1	0	2.431218	2.949551	0.677797
21	1	0	4.025934	2.564499	0.037961

TS: F_5P-F-CH_3 + 3-mt --> 1,3-dmt PF_6

Sum of electronic and zero-point Energies= -1572.526643 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1572.572467 (Hartree/particle)
1 imaginary frequency (544.9505i cm-1)
Standard orientation:

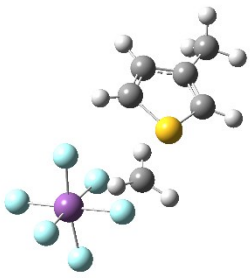
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.409886	-0.155752	-0.923311
2	6	0	3.491969	0.897307	-0.071975
3	6	0	3.042738	0.547586	1.257904
4	6	0	2.644788	-0.739055	1.373121
5	16	0	2.803278	-1.585326	-0.139320
6	1	0	3.022390	1.252180	2.080914
7	6	0	0.367476	-1.032793	-0.690782
8	1	0	0.072745	-1.709025	0.098421
9	1	0	0.693523	-0.029954	-0.455266
10	1	0	0.501422	-1.421651	-1.690178
11	9	0	-3.601395	-0.105935	-1.083880
12	9	0	-1.264877	0.385197	1.073955
13	9	0	-1.335785	-0.512086	-1.065810
14	9	0	-2.702237	-1.317942	0.621005
15	15	0	-2.489510	0.170121	0.041208
16	9	0	-3.551435	0.793549	1.058941
17	9	0	-2.170576	1.601984	-0.619540
18	1	0	3.672683	-0.193442	-1.971565
19	1	0	2.261102	-1.258148	2.240217
20	6	0	3.976482	2.266116	-0.439918
21	1	0	4.257171	2.315514	-1.492390
22	1	0	3.200147	3.012434	-0.253664
23	1	0	4.845748	2.542135	0.162229



TS: F_5Sb-F-CH_3 + 3-mt --> 1,3-dmt SbF_6

Sum of electronic and zero-point Energies= -1236.532057 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1236.580147 (Hartree/particle)
1 imaginary frequency (532.0790i cm-1)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.086389	-0.147827	-0.884077



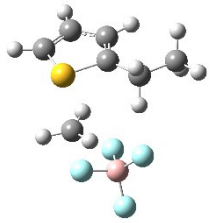
2	6	0	4.021212	0.909442	-0.039587
3	6	0	3.468128	0.594268	1.252624
4	6	0	3.114598	-0.704907	1.397626
5	16	0	3.461537	-1.581910	-0.086230
6	1	0	3.327288	1.325087	2.040380
7	6	0	1.067623	-1.074818	-0.803873
8	1	0	0.753673	-1.750703	-0.020588
9	1	0	1.373959	-0.066034	-0.565099
10	1	0	1.255792	-1.474781	-1.789773
11	9	0	-3.250148	-0.245861	-1.326395
12	9	0	-0.530414	0.356734	1.210003
13	9	0	-0.614665	-0.586063	-1.223697
14	9	0	-2.137404	-1.674579	0.643160
15	9	0	-3.262312	0.752394	1.254095
16	9	0	-1.659909	1.812218	-0.712732
17	51	0	-1.988704	0.107502	0.029198
18	1	0	2.688775	-1.132754	2.281098
19	1	0	4.461742	-0.114165	-1.885514
20	6	0	4.488797	2.319044	-0.447001
21	1	0	5.441901	2.253282	-0.928839
22	1	0	3.777667	2.749956	-1.120432
23	1	0	4.571702	2.933292	0.425195

TS: F_3B-F-CH_3 + 2-et --> 1m2-et BF_4

Sum of electronic and zero-point Energies= -1095.686836 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1095.730845 (Hartree/particle)
1 imaginary frequency (587.8660i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.000374	0.490256	-0.089273
2	6	0	2.213796	0.221510	1.221749
3	6	0	2.347489	-1.184026	1.515576
4	6	0	2.228533	-1.970034	0.422883
5	16	0	1.961212	-1.010980	-1.006249
6	1	0	2.269138	0.994368	1.978459
7	1	0	2.519559	-1.574573	2.510710
8	6	0	-0.496848	-1.046894	-0.860342
9	1	0	-0.525868	-2.067319	-1.213261
10	1	0	-0.332885	-0.847925	0.189928
11	1	0	-0.517197	-0.240621	-1.578130
12	6	0	1.771923	1.797857	-0.786775
13	1	0	0.813747	1.758733	-1.317896
14	1	0	2.540264	1.936104	-1.554094
15	9	0	-4.192143	0.259719	-0.194229
16	9	0	-2.749832	-0.329435	1.493907
17	9	0	-2.100494	1.207115	-0.075481
18	9	0	-2.333689	-1.002400	-0.669257
19	5	0	-2.879397	0.089640	0.183741
20	1	0	2.284495	-3.046469	0.344945
21	6	0	1.773721	2.980957	0.173847
22	1	0	2.731787	3.072526	0.690553
23	1	0	1.599257	3.907576	-0.375443
24	1	0	0.986789	2.882338	0.925042

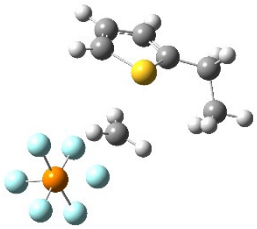


TS: F_5P-F-CH_3 + 2-et --> 1m2-et PF_6

Sum of electronic and zero-point Energies= -1611.801496 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1611.847978 (Hartree/particle)
1 imaginary frequency (542.8179i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.273780	0.105303	0.417416
2	6	0	3.069512	-0.838733	1.369619
3	6	0	2.501708	-2.063446	0.868259
4	6	0	2.280711	-2.034319	-0.465311
5	16	0	2.758454	-0.504432	-1.148215
6	1	0	3.318142	-0.673614	2.411265
7	1	0	2.267088	-2.918602	1.489515
8	6	0	0.346402	0.316868	-0.932227
9	1	0	0.063355	-0.463025	-1.623113
10	1	0	0.494031	0.086480	0.114765
11	1	0	0.647874	1.277843	-1.321284
12	6	0	3.851440	1.480935	0.555754
13	1	0	4.086034	1.626700	1.612945
14	1	0	4.798782	1.535769	0.010309
15	9	0	-1.912169	-1.325261	-0.360887
16	9	0	-3.247794	1.471087	0.508068
17	9	0	-1.362273	0.901388	-0.689855
18	9	0	-1.723586	0.055453	1.433849
19	15	0	-2.640951	0.038405	0.107732
20	9	0	-3.815226	-0.756075	0.843373
21	9	0	-3.441530	0.084104	-1.285696
22	1	0	1.859208	-2.796792	-1.105131
23	6	0	2.914370	2.586680	0.068658
24	1	0	3.361879	3.566780	0.244694
25	1	0	2.721475	2.506797	-1.005104
26	1	0	1.956787	2.550514	0.593935

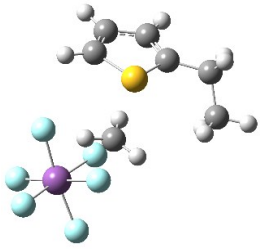


TS: F_5Sb-F-CH_3 + 2-et --> 1m2-et SbF_6

Sum of electronic and zero-point Energies= -1275.807628 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1275.857984 (Hartree/particle)
1 imaginary frequency (-527.4567 cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.889739	0.095352	0.442832
2	6	0	3.611154	-0.822918	1.401225
3	6	0	3.033160	-2.041619	0.895677
4	6	0	2.881613	-2.035623	-0.447408
5	16	0	3.437342	-0.533134	-1.135556
6	1	0	3.810230	-0.642492	2.450952
7	1	0	2.743181	-2.876380	1.521180
8	6	0	1.049289	0.339842	-1.027535
9	1	0	0.767671	-0.488683	-1.660226
10	1	0	1.186394	0.187478	0.034698
11	1	0	1.362058	1.266946	-1.484596
12	6	0	4.483785	1.463449	0.585207
13	1	0	4.697674	1.612643	1.646310
14	1	0	5.442539	1.504973	0.059089
15	9	0	-3.108584	1.646783	-0.110983



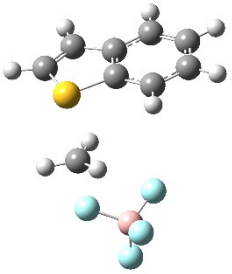
16	9	0	-0.996407	-1.465255	0.132284
17	9	0	-0.654588	0.932128	-0.834381
18	9	0	-2.739584	-0.508021	-1.644681
19	9	0	-3.571135	-0.870652	0.941640
20	9	0	-1.408796	0.643304	1.692309
21	51	0	-2.162506	0.025620	0.073252
22	1	0	2.470551	-2.799286	-1.092593
23	6	0	3.568463	2.577022	0.073581
24	1	0	4.022337	3.553147	0.255465
25	1	0	3.396509	2.494736	-1.003403
26	1	0	2.599807	2.552810	0.579015

TS: F_3B-F-CH_3 + bt --> 1-mbt BF_4

Sum of electronic and zero-point Energies= -1170.713807 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1170.759517 (Hartree/particle)
1 imaginary frequency (593.6362i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.787294	-0.028510	0.585814
2	6	0	-2.401413	0.015058	-0.676337
3	6	0	-2.458151	-1.291957	-1.302545
4	6	0	-1.910697	-2.264273	-0.551828
5	16	0	-1.293370	-1.670172	0.982557
6	1	0	-2.896567	-1.465399	-2.277810
7	6	0	1.039098	-1.305560	0.250900
8	1	0	1.211121	-2.370893	0.282999
9	1	0	0.601079	-0.856472	-0.629372
10	1	0	1.178172	-0.721410	1.149731
11	6	0	-1.601412	1.109553	1.365009
12	1	0	-1.122865	1.055976	2.336386
13	9	0	3.318688	0.648010	1.163296
14	9	0	4.484322	0.416450	-0.803298
15	9	0	2.325068	1.208152	-0.822049
16	9	0	2.741168	-1.000797	-0.333974
17	5	0	3.251350	0.395679	-0.194807
18	1	0	-1.821799	-3.318500	-0.774275
19	6	0	-2.054291	2.319432	0.856540
20	1	0	-1.922819	3.224148	1.438936
21	6	0	-2.855601	1.245879	-1.165132
22	1	0	-3.335883	1.299371	-2.136164
23	6	0	-2.678633	2.385180	-0.396551
24	1	0	-3.026114	3.342386	-0.768322

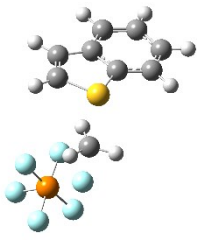


TS: F_5P-F-CH_3 + bt --> 1-mbt PF_6

Sum of electronic and zero-point Energies= -1686.827767 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1686.874826 (Hartree/particle)
1 imaginary frequency (547.9754i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.863907	-0.266213	-0.441560
2	6	0	2.882607	0.065967	0.923641



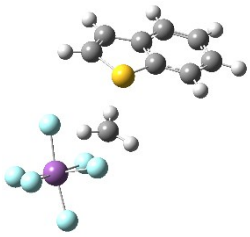
3	6	0	2.329380	-0.988304	1.750050
4	6	0	1.912639	-2.053068	1.040860
5	16	0	2.161593	-1.859751	-0.687069
6	1	0	2.255271	-0.923689	2.828689
7	6	0	-0.187471	-0.892843	-1.028128
8	1	0	-0.581227	-1.873559	-0.806011
9	1	0	0.121359	-0.237110	-0.225930
10	1	0	0.082645	-0.651283	-2.046127
11	9	0	-1.805228	1.327657	0.588342
12	9	0	-3.919886	-0.816944	-0.536361
13	9	0	-1.811286	-0.133500	-1.209958
14	9	0	-3.515310	1.388615	-0.912256
15	9	0	-3.922361	0.654860	1.256639
16	9	0	-2.202087	-0.878734	0.951763
17	1	0	1.463090	-2.967640	1.402174
18	6	0	3.328344	0.602790	-1.426199
19	6	0	3.856731	2.183646	0.338226
20	6	0	3.824840	1.833114	-1.019156
21	6	0	3.392084	1.312275	1.309751
22	1	0	3.415099	1.585112	2.359348
23	1	0	4.249031	3.151278	0.629804
24	1	0	4.194803	2.530612	-1.762073
25	1	0	3.307552	0.329078	-2.475346
26	15	0	-2.915072	0.276762	0.077343

TS: $F_5Sb\text{-}F\text{-}CH_3$ + bt --> 1-mbt SbF_6

Sum of electronic and zero-point Energies= -1350.833753 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1350.884054 (Hartree/particle)
1 imaginary frequency (529.9266i cm-1)

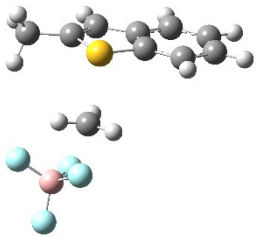
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.626172	-0.300633	-0.417103
2	6	0	3.611502	0.080542	0.935517
3	6	0	2.949165	-0.900873	1.771664
4	6	0	2.491471	-1.961504	1.081550
5	16	0	2.828782	-1.851694	-0.638481
6	1	0	2.829838	-0.789806	2.842507
7	6	0	0.559344	-0.752662	-1.076012
8	1	0	0.111884	-1.716772	-0.880257
9	1	0	0.873412	-0.124192	-0.255160
10	1	0	0.873352	-0.517770	-2.082810
11	9	0	-1.926169	1.937402	0.415662
12	9	0	-2.876943	-1.597747	-0.481035
13	9	0	-1.012079	0.090611	-1.269431
14	9	0	-3.574360	0.825558	-1.359092
15	9	0	-3.873166	0.215455	1.330401
16	9	0	-1.211636	-0.485526	1.267100
17	51	0	-2.498845	0.177114	0.046642
18	1	0	1.960914	-2.827753	1.452148
19	6	0	4.194800	0.494318	-1.409293
20	6	0	4.767005	2.096557	0.321572
21	6	0	4.764811	1.699085	-1.023263
22	6	0	4.197047	1.299495	1.300739
23	1	0	4.198147	1.608942	2.340353
24	1	0	5.221834	3.041463	0.596410
25	1	0	5.215613	2.339427	-1.772904
26	1	0	4.196859	0.183048	-2.448007



TS: $F_3B\text{-}F\text{-}CH_3$ + 2-mbt --> 1,2-dmbt BF_4

Sum of electronic and zero-point Energies= -1209.995418 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1210.042626 (Hartree/particle)
1 imaginary frequency (-583.3440 cm -1)

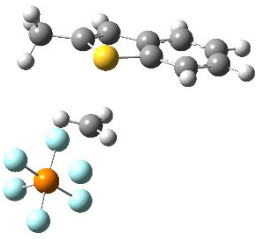


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.090710	-0.052028	-0.577936
2	6	0	-2.241841	0.141560	0.805108
3	6	0	-1.520957	1.307051	1.277611
4	6	0	-0.854519	1.972567	0.315111
5	16	0	-1.070990	1.203836	-1.268903
6	1	0	-1.507458	1.616372	2.316573
7	6	0	1.048856	-0.070793	-1.098291
8	1	0	1.574717	0.818968	-1.410495
9	1	0	0.765472	-0.204690	-0.062779
10	1	0	0.674012	-0.753344	-1.846962
11	6	0	-2.681426	-1.115896	-1.252263
12	1	0	-2.553863	-1.245601	-2.321292
13	9	0	2.769019	-1.139775	1.382826
14	9	0	4.642560	-1.310418	0.063401
15	9	0	3.545294	0.700958	0.263704
16	9	0	2.583120	-1.027226	-0.910439
17	5	0	3.438295	-0.678770	0.266018
18	6	0	-3.444586	-2.008307	-0.509849
19	1	0	-3.917197	-2.847566	-1.007168
20	6	0	-3.019014	-0.767844	1.530963
21	1	0	-3.149934	-0.635729	2.599667
22	6	0	-3.611638	-1.833420	0.869796
23	1	0	-4.212781	-2.542385	1.427806
24	6	0	0.024256	3.172288	0.424173
25	1	0	0.012986	3.539174	1.451026
26	1	0	1.057649	2.928245	0.159870
27	1	0	-0.309701	3.976084	-0.235861

TS: $F_5P\text{-}F\text{-}CH_3$ + 2-mbt --> 1,2-dmbt PF_6

Sum of electronic and zero-point Energies= -1726.109401 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1726.157813 (Hartree/particle)
1 imaginary frequency (544.5235i cm-1)



Standard orientation:

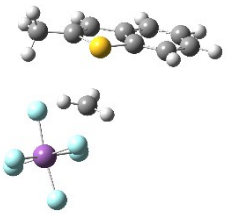
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.911604	-0.047217	-0.547409
2	6	0	-2.923154	0.009118	0.856519
3	6	0	-2.204712	1.159673	1.364729
4	6	0	-1.673785	1.945596	0.407159
5	16	0	-2.020381	1.313427	-1.213583
6	1	0	-2.093608	1.372221	2.421898
7	6	0	0.231641	0.087338	-1.170962
8	1	0	0.685772	1.065703	-1.235442
9	1	0	-0.152147	-0.274450	-0.228126

10	1	0	-0.029931	-0.427813	-2.084778
11	9	0	3.006836	1.116814	-0.496912
12	9	0	2.967980	-1.889850	0.638480
13	9	0	1.786556	-0.783394	-1.017532
14	9	0	1.879006	0.039787	1.151134
15	9	0	4.203100	0.007702	1.155597
16	9	0	4.095576	-0.812550	-1.016066
17	6	0	-3.527987	-1.073557	-1.257913
18	6	0	-4.200563	-2.028266	0.868549
19	6	0	-4.173299	-2.065955	-0.532043
20	6	0	-3.582951	-1.001864	1.566301
21	1	0	-3.604239	-0.975454	2.650432
22	1	0	-4.712374	-2.814711	1.411787
23	1	0	-4.663466	-2.877768	-1.057330
24	1	0	-3.508834	-1.097097	-2.341680
25	6	0	-0.850425	3.181701	0.543865
26	1	0	-0.736176	3.428355	1.599968
27	1	0	0.147235	3.044350	0.115587
28	1	0	-1.316754	4.029928	0.037159
29	15	0	3.050678	-0.372938	0.120184

TS: $F_5Sb\text{-}F\text{-}CH_3$ + 2-mbt --> 1,2-dmbt SbF_6

Sum of electronic and zero-point Energies= -1390.115893 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1390.167771 (Hartree/particle)
1 imaginary frequency (530.9158i cm-1)

Standard orientation:



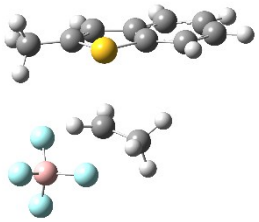
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.562421	-0.057140	-0.519261
2	6	0	-3.473997	-0.116290	0.882037
3	6	0	-2.785308	1.031498	1.436254
4	6	0	-2.373687	1.925261	0.515208
5	16	0	-2.800757	1.405820	-1.126112
6	1	0	-2.605742	1.163235	2.497150
7	6	0	-0.482589	0.342976	-1.319681
8	1	0	-0.101807	1.351997	-1.383245
9	1	0	-0.763783	-0.072778	-0.362354
10	1	0	-0.783840	-0.160062	-2.227400
11	9	0	3.124600	1.286010	-0.880070
12	9	0	1.782575	-1.770425	0.869757
13	9	0	1.133546	-0.408781	-1.318037
14	9	0	1.279886	0.836110	0.975004
15	9	0	3.862147	-0.053567	1.401020
16	9	0	3.603938	-1.337978	-1.038295
17	6	0	-4.175474	-1.055170	-1.271386
18	6	0	-4.639402	-2.218335	0.805995
19	6	0	-4.713292	-2.139523	-0.591239
20	6	0	-4.026970	-1.218387	1.545495
21	1	0	-3.971902	-1.281989	2.627002
22	1	0	-5.070318	-3.073902	1.313610
23	1	0	-5.198845	-2.932166	-1.149047
24	1	0	-4.235757	-0.987734	-2.352019
25	6	0	-1.624511	3.201814	0.699982
26	1	0	-0.696544	3.210732	0.121206
27	1	0	-2.220980	4.060873	0.382477
28	1	0	-1.371451	3.327154	1.753345
29	51	0	2.547035	-0.240020	0.070828

TS: $F_5Sb\text{-}F\text{-}CH_2\text{-}CH_3$ + 2-mbt --> 1e2-mbt BF4

Sum of electronic and zero-point Energies= -1249.280310 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1249.329129 (Hartree/particle)
1 imaginary frequency (403.7019i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.246727	0.037412	-0.469252
2	6	0	-2.199085	0.562562	0.834840
3	6	0	-1.232107	1.633361	0.955630
4	6	0	-0.577123	1.913788	-0.190023
5	16	0	-1.104558	0.861682	-1.512617
6	1	0	-1.039982	2.161909	1.882362
7	6	0	0.891263	-0.810666	-0.811265
8	1	0	1.491053	-0.081924	-1.339255
9	1	0	0.522333	-0.542662	0.170808
10	6	0	-3.096702	-1.008644	-0.820474
11	1	0	-3.123134	-1.394094	-1.833761
12	9	0	3.959594	0.239844	-0.605040
13	9	0	2.634610	0.509237	1.243029
14	9	0	4.396987	-0.967229	1.302229
15	9	0	2.539459	-1.445062	0.040439
16	5	0	3.425629	-0.376251	0.519395
17	6	0	-3.917204	-1.537402	0.167344
18	1	0	-4.588641	-2.352451	-0.077681
19	6	0	-3.040034	0.015447	1.811987
20	1	0	-3.020920	0.407402	2.823186
21	6	0	-3.888858	-1.026966	1.472171
22	1	0	-4.542190	-1.453602	2.224919
23	6	0	0.489028	2.924778	-0.449394
24	1	0	0.157616	3.669079	-1.177864
25	1	0	0.742286	3.436758	0.479489
26	1	0	1.397534	2.458663	-0.840640
27	6	0	0.445275	-2.050281	-1.461677
28	1	0	-0.620651	-2.210654	-1.280767
29	1	0	0.674825	-2.069872	-2.524418
30	1	0	0.952444	-2.885649	-0.966712

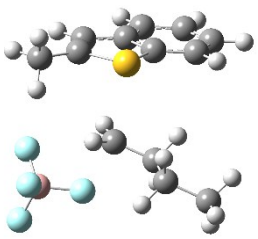


TS: $F_5Sb\text{-}F\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$ + 2-mbt --> 1e2-mbt BF_4

Sum of electronic and zero-point Energies= -1327.830369 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1327.883504 (Hartree/particle)
1 imaginary frequency (367.1129i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.353120	0.017231	0.370808
2	6	0	-2.407979	-1.189591	-0.349742
3	6	0	-1.499063	-2.183464	0.180706
4	6	0	-0.787039	-1.763293	1.246601
5	16	0	-1.184273	-0.091718	1.673312
6	1	0	-1.385735	-3.174914	-0.242609
7	6	0	0.849166	0.613323	0.026918
8	1	0	1.428656	0.295897	0.885318



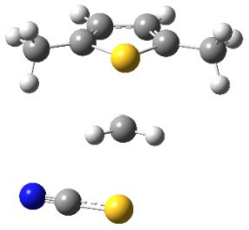
9	1	0	0.383459	-0.152772	-0.582481
10	6	0	-3.133725	1.121379	0.035207
11	1	0	-3.085781	2.039237	0.610952
12	9	0	3.697614	-0.718778	0.574482
13	9	0	2.341229	-1.879230	-0.860608
14	9	0	4.289469	-0.934558	-1.636879
15	9	0	2.517291	0.401454	-1.042386
16	5	0	3.246548	-0.829619	-0.736870
17	6	0	-3.985377	1.006493	-1.055734
18	1	0	-4.604600	1.849956	-1.339237
19	6	0	-3.277330	-1.281227	-1.443731
20	1	0	-3.334465	-2.203398	-2.012214
21	6	0	-4.055260	-0.186263	-1.788262
22	1	0	-4.729077	-0.252231	-2.635066
23	6	0	0.261558	-2.481462	2.027876
24	1	0	-0.024358	-2.584859	3.077547
25	1	0	0.412628	-3.476589	1.608134
26	1	0	1.216143	-1.948457	1.993814
27	6	0	0.588105	2.032296	-0.238521
28	1	0	-0.501868	2.165471	-0.282205
29	1	0	0.902160	2.209301	-1.276643
30	6	0	1.251981	3.001837	0.730076
31	1	0	2.330363	2.817197	0.732960
32	1	0	0.891234	2.800391	1.743825
33	6	0	0.968423	4.449677	0.351243
34	1	0	1.436627	5.140248	1.055346
35	1	0	1.353845	4.675915	-0.646518
36	1	0	-0.106077	4.653567	0.348297

TS: NCS-CH_3 + 2,5- dmt --> 1,2,5-tmt NCS

Sum of electronic and zero-point Energies= -1162.273053 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1162.316901 (Hartree/particle)
One imaginary frequency (539.7423 cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.165057	-0.928098	0.272815
2	6	0	-2.409905	-0.097683	1.307920
3	6	0	-1.948222	1.259044	1.105854
4	6	0	-1.350074	1.470790	-0.084904
5	16	0	-1.360440	-0.029553	-1.015538
6	1	0	-2.905005	-0.430217	2.212739
7	1	0	-2.059158	2.042048	1.846740
8	6	0	0.722306	-0.640310	-0.564972
9	1	0	1.168414	0.060751	-1.255165
10	1	0	0.632094	-0.390829	0.482719
11	1	0	0.594317	-1.664550	-0.884643
12	6	0	-2.447469	-2.382987	0.106980
13	1	0	-3.086697	-2.574303	-0.757867
14	1	0	-1.524555	-2.954583	-0.026401
15	1	0	-2.952418	-2.756176	0.998848
16	6	0	-0.707966	2.693841	-0.646468
17	1	0	-0.808183	3.512419	0.067283
18	1	0	0.358334	2.533148	-0.831940
19	1	0	-1.171422	2.996084	-1.588367
20	16	0	3.094369	-1.262520	0.003043
21	6	0	3.419531	0.326471	0.392559
22	7	0	3.618936	1.441850	0.656752



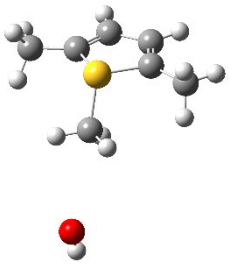
Solvolysis

Basic aqueous

Thiophenium cations + nucleophile

1,2,5-tmt OH (in water)

Sum of electronic and zero-point Energies= -747.031515 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.071167 (Hartree/particle)
No imaginary frequencies

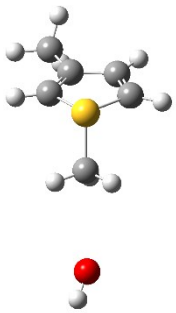


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.032975	1.301232	0.063423
2	6	0	1.868933	0.730345	0.940553
3	6	0	1.869367	-0.729540	0.940485
4	6	0	1.033749	-1.300843	0.063294
5	16	0	0.265284	0.000004	-0.898132
6	1	0	2.482195	1.316817	1.614203
7	1	0	2.483008	-1.315755	1.614018
8	6	0	-1.442808	-0.000499	-0.269279
9	1	0	-1.922145	-0.894181	-0.664243
10	1	0	-1.410568	-0.000648	0.817695
11	1	0	-1.922562	0.893079	-0.663994
12	6	0	0.696306	2.720424	-0.223494
13	1	0	-0.364523	2.915097	-0.044812
14	1	0	1.282753	3.360060	0.436520
15	1	0	0.921187	2.984238	-1.258903
16	6	0	0.697994	-2.720226	-0.223789
17	1	0	1.284676	-3.359551	0.436313
18	1	0	-0.362762	-2.915546	-0.045378
19	1	0	0.923274	-2.983839	-1.259165
20	8	0	-4.636657	0.001370	0.532005
21	1	0	-5.084916	-0.016155	1.384658

1,3-dmt OH (in water)

Sum of electronic and zero-point Energies= -707.748375 (Hartree/particle)
Sum of electronic and thermal Free Energies= -707.786623 (Hartree/particle)
No imaginary frequencies



Standard orientation:

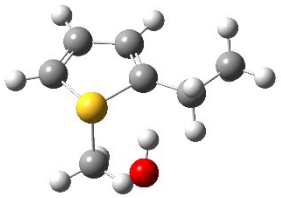
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.938786	0.516695	-0.905940
2	6	0	-1.856154	0.480632	0.072449
3	6	0	-1.638187	-0.626235	1.017233
4	6	0	-0.585114	-1.396844	0.737257
5	16	0	0.158740	-0.860991	-0.778913
6	1	0	-2.280971	-0.786371	1.874689
7	1	0	-0.184646	-2.266026	1.239365
8	6	0	1.731687	-0.124303	-0.223324
9	1	0	2.381433	-0.953563	0.048192

10	1	0	2.137105	0.416198	-1.075775
11	1	0	1.525998	0.531172	0.619193
12	6	0	-2.983308	1.443695	0.230559
13	1	0	-3.935207	0.908173	0.205557
14	1	0	-2.912784	1.941407	1.200698
15	1	0	-2.974410	2.194195	-0.558435
16	1	0	-0.835136	1.190176	-1.745034
17	8	0	4.584862	0.949946	0.588661
18	1	0	5.479052	1.239094	0.375472

1m2-et OH (in water)

Sum of electronic and zero-point Energies= -747.024348 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.047363 (Hartree/particle)
No imaginary frequencies

Standard orientation:

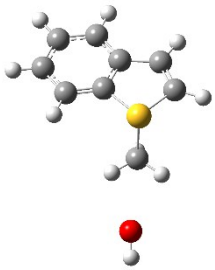


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.229079	-0.713690	-0.100626
2	6	0	-0.626368	-1.746553	-0.112200
3	6	0	-2.035563	-1.378461	-0.219615
4	6	0	-2.252640	-0.060735	-0.280868
5	16	0	-0.707947	0.803425	-0.316087
6	1	0	-0.299672	-2.775860	-0.031333
7	1	0	-2.833456	-2.110230	-0.237116
8	1	0	-3.171663	0.500635	-0.367416
9	6	0	1.715411	-0.650969	0.015916
10	1	0	2.126057	-0.213815	-0.899599
11	1	0	1.980511	0.035096	0.827324
12	6	0	2.320406	-2.027735	0.264223
13	1	0	3.404151	-1.943287	0.351342
14	1	0	1.937972	-2.466838	1.188016
15	1	0	2.098896	-2.710527	-0.558560
16	6	0	-0.636972	1.528586	1.350612
17	1	0	-1.333674	2.364777	1.359593
18	1	0	-0.914411	0.761349	2.069983
19	1	0	0.383296	1.881612	1.479074
20	8	0	1.744183	2.755982	-0.550077
21	1	0	1.715557	2.071764	-1.227958

1-mbt OH (in water)

Sum of electronic and zero-point Energies= -822.049859 (Hartree/particle)
Sum of electronic and thermal Free Energies= -822.080955 (Hartree/particle)
No imaginary frequencies

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.323467	0.604703	0.504740
2	6	0	0.632040	-0.072993	-0.504101
3	6	0	1.007290	-1.308210	-0.996474
4	6	0	2.138148	-1.892201	-0.426211
5	6	0	2.850577	-1.239921	0.580546
6	6	0	2.455637	0.009347	1.051928
7	6	0	0.708834	1.886486	0.847105
8	6	0	-0.394172	2.173283	0.153340
9	1	0	0.455577	-1.803358	-1.786805

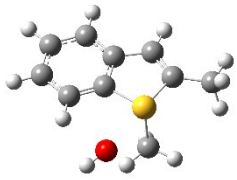
10	1	0	2.466660	-2.862615	-0.778046
11	1	0	3.729106	-1.714199	1.001544
12	1	0	3.012572	0.513868	1.832836
13	1	0	1.114268	2.546475	1.604453
14	1	0	-1.039996	3.038718	0.185464
15	16	0	-0.751664	0.906566	-1.049130
16	6	0	-2.165423	0.029577	-0.308325
17	1	0	-1.941119	-0.166024	0.737312
18	1	0	-2.291268	-0.888083	-0.880037
19	1	0	-3.032345	0.676765	-0.426557
20	8	0	-4.543985	-1.624118	1.094920
21	1	0	-5.433337	-1.994093	1.121275

1,2-dmbt OH in water

Sum of electronic and zero-point Energies= -861.334373 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.362566 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.832770	-1.172270	-0.057796
2	6	0	-0.596478	0.207534	-0.100861
3	6	0	-1.606295	1.150062	-0.039271
4	6	0	-2.913215	0.678016	0.079157
5	6	0	-3.177604	-0.691094	0.116385
6	6	0	-2.146187	-1.623254	0.046935
7	6	0	0.392038	-1.965081	-0.115059
8	6	0	1.517284	-1.247209	-0.183955
9	1	0	-1.380583	2.206931	-0.085626
10	1	0	-3.730068	1.387586	0.137395
11	1	0	-4.201792	-1.035521	0.201243
12	1	0	-2.353398	-2.686911	0.075879
13	1	0	0.386401	-3.048929	-0.088605
14	16	0	1.149675	0.519344	-0.290963
15	6	0	1.659579	1.018589	1.379399
16	1	0	2.747838	1.063606	1.377861
17	1	0	1.290271	0.283717	2.091827
18	1	0	1.237140	2.005633	1.539093
19	6	0	2.943537	-1.668718	-0.224679
20	1	0	3.491810	-1.279107	0.637829
21	1	0	2.999894	-2.757358	-0.206654
22	1	0	3.439225	-1.306389	-1.128387
23	8	0	0.749589	3.133795	-0.657985
24	1	0	0.242418	3.667433	-0.034087

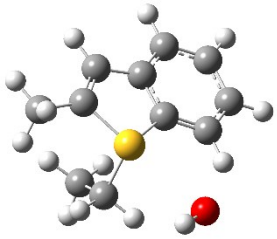


1e2-mbt OH in water

Sum of electronic and zero-point Energies= -900.613943 (Hartree/particle)
Sum of electronic and thermal Free Energies= -900.654818 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.952611	-1.196196	-0.164621
2	6	0	0.713704	0.180853	-0.248523



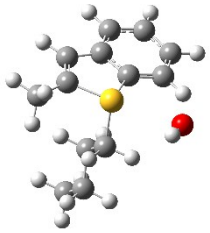
3	6	0	1.703535	1.135926	-0.108265
4	6	0	2.997732	0.675503	0.134613
5	6	0	3.267442	-0.690919	0.214778
6	6	0	2.254228	-1.634420	0.064414
7	6	0	-0.260345	-1.995607	-0.318425
8	6	0	-1.378486	-1.286706	-0.506167
9	1	0	1.462213	2.188030	-0.189881
10	1	0	3.801113	1.392431	0.255789
11	1	0	4.282609	-1.024532	0.396560
12	1	0	2.467156	-2.695434	0.127757
13	1	0	-0.255795	-3.078688	-0.268565
14	16	0	-1.004794	0.473521	-0.601301
15	6	0	-1.710161	1.069997	0.998093
16	1	0	-2.779085	1.148826	0.790754
17	1	0	-1.290805	2.071734	1.070622
18	6	0	-2.797032	-1.711737	-0.643981
19	1	0	-3.216757	-1.395841	-1.601851
20	1	0	-2.856869	-2.798103	-0.574133
21	1	0	-3.412531	-1.278526	0.150788
22	6	0	-1.399502	0.187096	2.183316
23	1	0	-1.794374	0.683564	3.072544
24	1	0	-1.872749	-0.792143	2.105457
25	1	0	-0.324720	0.058186	2.325289
26	8	0	-0.362112	3.274373	-0.827719
27	1	0	-1.298158	3.346430	-1.049947

1b2-mbt OH (in water)

Sum of electronic and zero-point Energies= -979.158770 (Hartree/particle)
Sum of electronic and thermal Free Energies= -979.202416 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.515615	0.310487	-1.067049
2	6	0	1.222755	0.027478	0.273286
3	6	0	1.860762	-0.964135	0.995965
4	6	0	2.831234	-1.711534	0.328808
5	6	0	3.147481	-1.447323	-1.004067
6	6	0	2.498961	-0.437065	-1.709405
7	6	0	0.696040	1.386085	-1.617983
8	6	0	-0.193194	1.902325	-0.764350
9	1	0	1.607651	-1.135800	2.033685
10	1	0	3.348070	-2.502781	0.858995
11	1	0	3.911775	-2.036334	-1.497795
12	1	0	2.747146	-0.231474	-2.744553
13	1	0	0.791356	1.726657	-2.642891
14	16	0	-0.016905	1.158647	0.867339
15	6	0	-1.577185	0.182128	0.963107
16	1	0	-2.342896	0.951003	1.095466
17	1	0	-1.460616	-0.364074	1.897883
18	6	0	-1.234838	2.946633	-0.954073
19	1	0	-1.124352	3.758923	-0.232273
20	1	0	-1.153334	3.357249	-1.960825
21	1	0	-2.236917	2.523206	-0.833305
22	6	0	-1.843375	-0.710698	-0.230724
23	1	0	-1.901758	-0.118154	-1.148346
24	1	0	-1.027805	-1.430563	-0.350251
25	8	0	0.407789	0.108573	3.446968



26	1	0	-0.171642	0.824674	3.733675
27	6	0	-3.160610	-1.462327	-0.026926
28	1	0	-3.970800	-0.738938	0.108706
29	1	0	-3.104837	-2.049949	0.894618
30	6	0	-3.471900	-2.374355	-1.207571
31	1	0	-2.690276	-3.127201	-1.340038
32	1	0	-4.419505	-2.897892	-1.063842
33	1	0	-3.543555	-1.801692	-2.136183

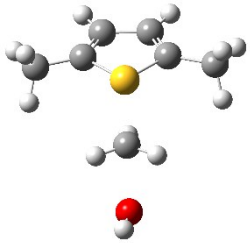
TS basic hydrolysis

TS: 1,2,5-tmt OH --> 2,5-dmt + CH_3OH (in water)

Sum of electronic and zero-point Energies= -747.016431 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.053503 (Hartree/particle)
1 imaginary frequency (613.5808i) cm-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.935928	1.278443	0.025380
2	6	0	1.677416	0.717165	1.000110
3	6	0	1.669600	-0.732654	1.000957
4	6	0	0.921873	-1.287079	0.027016
5	16	0	0.207968	-0.001019	-0.957442
6	1	0	2.224679	1.308545	1.724430
7	1	0	2.210941	-1.329039	1.725622
8	6	0	-1.738398	0.012579	-0.127730
9	1	0	-2.073868	-0.915451	-0.565191
10	1	0	-1.434227	0.020302	0.908441
11	1	0	-2.067843	0.934261	-0.582217
12	6	0	0.664115	2.707925	-0.294195
13	1	0	-0.406833	2.925478	-0.258832
14	1	0	1.167874	3.340723	0.437009
15	1	0	1.026387	2.970998	-1.290363
16	6	0	0.636886	-2.714038	-0.292393
17	1	0	1.133620	-3.351414	0.439647
18	1	0	-0.436001	-2.921777	-0.258537
19	1	0	0.998140	-2.980772	-1.287961
20	8	0	-3.747808	0.028353	0.786237
21	1	0	-4.292413	-0.106416	0.002262

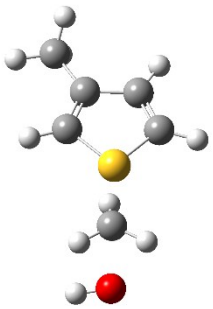


TS: 1,3-dmt OH --> 3-mt + CH_3OH (in water)

Sum of electronic and zero-point Energies= -707.734472 (Hartree/particle)
Sum of electronic and thermal Free Energies= -707.769879 (Hartree/particle)
1 imaginary frequency (595.8473i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.857259	0.278856	-1.014165
2	6	0	-1.719839	0.442634	0.009733
3	6	0	-1.478058	-0.506401	1.090751
4	6	0	-0.457862	-1.348995	0.859549
5	16	0	0.249295	-1.045339	-0.716327
6	1	0	-2.068300	-0.520389	1.999240
7	1	0	-0.055469	-2.137723	1.478796
8	6	0	1.970370	0.023477	-0.113008



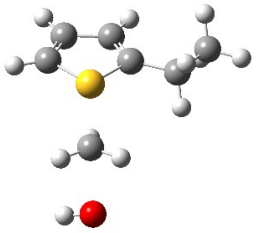
9	1	0	2.515254	-0.809004	0.304194
10	1	0	2.264084	0.374508	-1.090301
11	1	0	1.464047	0.701638	0.556616
12	6	0	-2.802039	1.470932	0.071330
13	1	0	-3.776600	0.990834	0.187562
14	1	0	-2.654519	2.121241	0.937012
15	1	0	-2.816940	2.084124	-0.829177
16	1	0	-0.788084	0.828238	-1.942382
17	8	0	3.776335	1.133058	0.562494
18	1	0	3.785245	1.864466	-0.065424

TS: 2e1-mt OH --> 2-et + CH_3OH (in water)

Sum of electronic and zero-point Energies= -747.008983 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.060986 (Hartree/particle)
1 imaginary frequency (602.7515i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.014856	-0.042338	-0.143982
2	6	0	-1.427115	0.786788	0.836627
3	6	0	-0.677709	2.026506	0.919539
4	6	0	0.301884	2.127209	0.003247
5	16	0	0.318016	0.714269	-1.031046
6	1	0	-2.237766	0.541913	1.511628
7	1	0	-0.882535	2.797060	1.651804
8	1	0	1.007088	2.926325	-0.173892
9	6	0	-1.462735	-1.416376	-0.528238
10	1	0	-1.736934	-1.423523	-1.587427
11	1	0	-0.613840	-2.102721	-0.426568
12	6	0	-2.630416	-1.902680	0.320765
13	1	0	-2.922043	-2.907379	0.012237
14	1	0	-2.363656	-1.937815	1.379107
15	1	0	-3.497692	-1.248563	0.208554
16	6	0	1.901625	-0.393310	-0.181683
17	1	0	2.712008	0.234187	-0.518666
18	1	0	1.570619	-0.316351	0.842884
19	1	0	1.724521	-1.313099	-0.718385
20	8	0	3.527736	-1.607563	0.715996
21	1	0	3.986025	-0.932622	1.229843

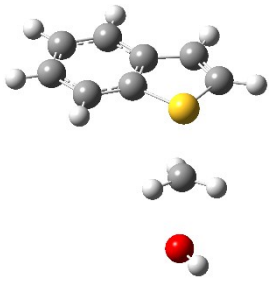


TS: 1-mbt OH --> bt + CH_3OH (in water)

Sum of electronic and zero-point Energies= -822.035217 (Hartree/particle)
Sum of electronic and thermal Free Energies= -822.071910 (Hartree/particle)
1 imaginary frequency (599.6117i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.200326	0.741322	0.421703
2	6	0	0.567059	-0.065870	-0.533320
3	6	0	1.072538	-1.291944	-0.940355
4	6	0	2.266309	-1.712469	-0.362736
5	6	0	2.923174	-0.921252	0.585267
6	6	0	2.401271	0.302950	0.982762
7	6	0	0.457950	1.964324	0.690040
8	6	0	-0.674352	2.073792	-0.019235



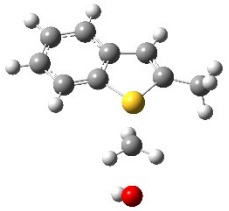
9	1	0	0.564563	-1.897889	-1.681492
10	1	0	2.692396	-2.664262	-0.657343
11	1	0	3.854601	-1.270219	1.015788
12	1	0	2.910851	0.914122	1.719000
13	1	0	0.791467	2.713758	1.397291
14	1	0	-1.407957	2.867445	-0.020467
15	16	0	-0.923307	0.695565	-1.095231
16	6	0	-2.332594	-0.428868	0.016713
17	1	0	-1.854230	-0.311835	0.977226
18	1	0	-2.203200	-1.354978	-0.522283
19	1	0	-3.196049	0.177432	-0.211034
20	8	0	-3.762360	-1.596918	1.219778
21	1	0	-4.570735	-1.499184	0.703760

TS: 1,2-dmbt OH --> 2-mbt + CH_3OH (in water)

Sum of electronic and zero-point Energies= -861.303899 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.342852 (Hartree/particle)
1 imaginary frequency (468.3193i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.221255	0.773083	0.408258
2	6	0	0.796302	-0.186831	-0.519913
3	6	0	1.576740	-1.264264	-0.908447
4	6	0	2.839537	-1.377693	-0.332970
5	6	0	3.291584	-0.430213	0.589155
6	6	0	2.494855	0.646129	0.963705
7	6	0	0.209869	1.790198	0.659493
8	6	0	-0.932122	1.631176	-0.026126
9	1	0	1.221667	-1.991511	-1.629580
10	1	0	3.476127	-2.210439	-0.608134
11	1	0	4.280401	-0.537223	1.020665
12	1	0	2.852231	1.377707	1.679993
13	1	0	0.358648	2.608437	1.354922
14	16	0	-0.837284	0.189721	-1.080588
15	6	0	-1.936265	-1.121956	-0.013411
16	1	0	-2.933098	-0.737858	-0.169844
17	1	0	-1.509916	-0.986758	0.970766
18	1	0	-1.704720	-2.043919	-0.525182
19	6	0	-2.190000	2.427310	-0.019412
20	1	0	-3.045404	1.813552	0.276298
21	1	0	-2.092587	3.246579	0.693422
22	1	0	-2.401285	2.845133	-1.006673
23	8	0	-3.293658	-2.610231	1.061124
24	1	0	-2.986779	-2.859021	1.941772

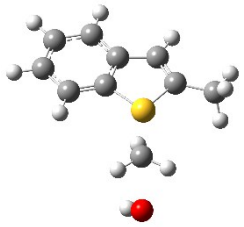


TS: 1e2-mbt OH --> 2-mbt + CH_3CH_2OH (in water)

Sum of electronic and zero-point Energies= -900.593185 (Hartree/particle)
Sum of electronic and thermal Free Energies= -900.633269 (Hartree/particle)
1 imaginary frequency (554.9707 i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.502599	0.691525	0.331974



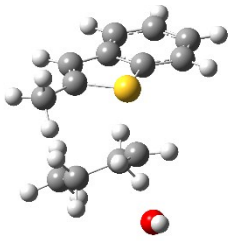
2	6	0	-0.954201	-0.221918	-0.581498
3	6	0	-1.587126	-1.406295	-0.933560
4	6	0	-2.818657	-1.675051	-0.344677
5	6	0	-3.389446	-0.776151	0.562570
6	6	0	-2.742680	0.404714	0.905461
7	6	0	-0.636474	1.837202	0.556408
8	6	0	0.510386	1.811739	-0.142989
9	1	0	-1.143102	-2.096904	-1.641357
10	1	0	-3.340358	-2.590657	-0.597062
11	1	0	-4.351818	-1.006161	1.005195
12	1	0	-3.186520	1.097768	1.611474
13	1	0	-0.886607	2.643416	1.236251
14	16	0	0.601384	0.358775	-1.164293
15	6	0	2.057137	-0.881184	-0.038838
16	1	0	2.891639	-0.342876	-0.460748
17	1	0	1.750576	-1.781671	-0.551503
18	6	0	1.658101	2.760006	-0.147379
19	1	0	1.826953	3.177343	-1.142548
20	1	0	1.455422	3.577627	0.544771
21	1	0	2.579539	2.260056	0.166656
22	6	0	1.650741	-0.663241	1.382929
23	1	0	2.138937	-1.427720	1.987272
24	1	0	1.960125	0.316433	1.746277
25	1	0	0.573773	-0.780653	1.522150
26	8	0	3.794286	-2.216534	0.524590
27	1	0	4.283923	-2.342200	-0.297260

TS: 1b2-mbt OH --> 2-mbt + $CH_3CH_2CH_2CH_2OH$ (in water)

Sum of electronic and zero-point Energies= -979.140332 (Hartree/particle)
Sum of electronic and thermal Free Energies= -979.184723 (Hartree/particle)
1 imaginary frequency (527.6030i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.409365	-0.253878	-0.691783
2	6	0	-1.693366	0.724488	0.273271
3	6	0	-0.765986	1.843338	0.218155
4	6	0	0.174223	1.739722	-0.736449
5	16	0	-0.009463	0.219528	-1.645118
6	1	0	-0.828557	2.696298	0.884396
7	6	0	1.622408	-0.993974	-0.774065
8	1	0	1.283997	-1.886066	-1.281806
9	1	0	2.378700	-0.412010	-1.283090
10	6	0	-2.135345	-1.431799	-0.806606
11	1	0	-1.891712	-2.176044	-1.556146
12	6	0	-3.193510	-1.620991	0.076439
13	1	0	-3.781912	-2.528897	0.015136
14	6	0	-2.764274	0.516668	1.144727
15	1	0	-3.004000	1.260792	1.896011
16	6	0	-3.504737	-0.653927	1.038149
17	1	0	-4.334883	-0.824520	1.713826
18	6	0	1.265902	2.676644	-1.124541
19	1	0	1.349459	3.467144	-0.377869
20	1	0	2.229136	2.165386	-1.198840
21	1	0	1.058566	3.133534	-2.095462
22	6	0	1.453667	-0.880016	0.713203
23	1	0	0.408229	-0.676009	0.968999
24	1	0	1.656860	-1.871131	1.126766



25	6	0	2.354050	0.160821	1.372047
26	1	0	2.241860	1.125417	0.869377
27	1	0	3.398614	-0.138239	1.251532
28	6	0	2.017469	0.320328	2.849554
29	1	0	2.682192	1.039108	3.333299
30	1	0	0.989951	0.674613	2.977592
31	1	0	2.110401	-0.631455	3.379885
32	8	0	3.481583	-2.311404	-0.523669
33	1	0	3.825022	-2.323694	-1.424986

Neutral aqueous

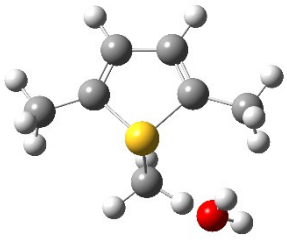
Thiophenium cations +1H_2O

1,2,5-tmt H_2O (in water)

Sum of electronic and zero-point Energies= -747.509035 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.545989 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.493806	1.208142	0.015610
2	6	0	0.627297	1.939369	0.083976
3	6	0	1.872987	1.188551	-0.032127
4	6	0	1.720545	-0.132626	-0.188867
5	16	0	-0.029786	-0.495136	-0.301785
6	1	0	0.601823	3.012419	0.232194
7	1	0	2.848039	1.657362	0.025100
8	6	0	-0.326411	-1.292151	1.304319
9	1	0	0.046069	-2.312032	1.226331
10	1	0	0.198958	-0.728074	2.071855
11	1	0	-1.401956	-1.291616	1.457584
12	6	0	-1.925040	1.600295	0.109020
13	1	0	-2.439037	1.053104	0.902684
14	1	0	-1.974685	2.666700	0.332369
15	1	0	-2.452275	1.413574	-0.828565
16	6	0	2.702588	-1.243141	-0.305615
17	1	0	3.710040	-0.836213	-0.215779
18	1	0	2.556615	-1.984073	0.485341
19	1	0	2.613634	-1.753609	-1.267007
20	8	0	-2.803128	-1.336102	-0.544181
21	1	0	-3.086729	-0.847306	-1.325156
22	1	0	-3.387857	-1.049878	0.167152

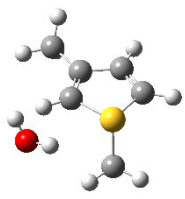


1,3-dmt H_2O (in water)

Sum of electronic and zero-point Energies= -708.225930 (Hartree/particle)
Sum of electronic and thermal Free Energies= -708.262331 (Hartree/particle)
No imaginary frequencies

Standard orientation:

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



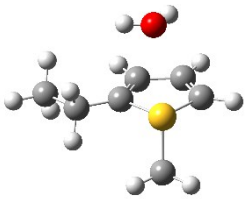
1	6	0	0.194176	0.028801	-0.951400
2	6	0	0.820822	0.933347	-0.183762
3	6	0	-0.074831	1.565152	0.798777
4	6	0	-1.337607	1.135729	0.757499
5	16	0	-1.529246	-0.027447	-0.567137
6	1	0	0.276501	2.308363	1.504517
7	1	0	-2.204101	1.408439	1.342590
8	6	0	-1.698059	-1.606771	0.326147
9	1	0	-2.709295	-1.634629	0.727183
10	1	0	-1.558046	-2.397796	-0.407807
11	1	0	-0.947674	-1.638433	1.113091
12	6	0	2.269061	1.276487	-0.264751
13	1	0	2.388617	2.340494	-0.483119
14	1	0	2.748262	1.087400	0.699198
15	1	0	2.772977	0.696378	-1.037100
16	1	0	0.568190	-0.584393	-1.759644
17	8	0	2.270167	-2.194485	0.506679
18	1	0	2.595122	-1.602269	-0.181314
19	1	0	1.334682	-1.985002	0.608101

2e1-mt H_2O (in water)

Sum of electronic and zero-point Energies= -747.501120 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.539068 (Hartree/particle)
No imaginary frequencies

Standard orientation:

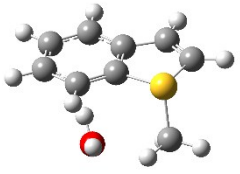
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.622053	0.087006	-0.143017
2	6	0	0.360761	-0.562178	-1.285565
3	6	0	-1.059709	-0.710222	-1.594863
4	6	0	-1.881633	-0.166360	-0.691526
5	16	0	-0.936658	0.512906	0.643292
6	1	0	1.139344	-0.941392	-1.935876
7	1	0	-1.415159	-1.212345	-2.485935
8	1	0	-2.960091	-0.119127	-0.649715
9	6	0	1.894706	0.452690	0.543509
10	1	0	1.879827	1.522545	0.779895
11	1	0	1.939404	-0.074637	1.502474
12	6	0	3.115781	0.118433	-0.304136
13	1	0	4.022724	0.410694	0.226166
14	1	0	3.173260	-0.952559	-0.508392
15	1	0	3.091077	0.650510	-1.257192
16	6	0	-1.012875	2.297503	0.288183
17	1	0	-2.020251	2.626007	0.535671
18	1	0	-0.288611	2.778876	0.943490
19	1	0	-0.782091	2.458504	-0.762400
20	8	0	-0.569015	-2.414679	1.334843
21	1	0	-0.867624	-2.767874	0.488937
22	1	0	0.392332	-2.369502	1.275955



1-mbt H_2O (in water)

Sum of electronic and zero-point Energies= -822.528757 (Hartree/particle)
Sum of electronic and thermal Free Energies= -822.566209 (Hartree/particle)
No imaginary frequencies

Standard orientation:

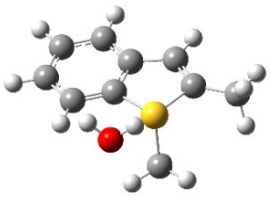


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.375658	-1.095571	0.244378
2	6	0	-0.016588	-0.077344	-0.643684
3	6	0	-0.927614	0.707818	-1.325025
4	6	0	-2.277552	0.456683	-1.079253
5	6	0	-2.668461	-0.553234	-0.198947
6	6	0	-1.728450	-1.337448	0.466011
7	6	0	0.782712	-1.761391	0.838092
8	6	0	1.961639	-1.278127	0.441178
9	1	0	-0.614562	1.483125	-2.014308
10	1	0	-3.028183	1.052336	-1.584378
11	1	0	-3.723798	-0.731701	-0.029804
12	1	0	-2.037498	-2.123313	1.145202
13	1	0	0.689388	-2.573456	1.549091
14	1	0	2.967631	-1.572593	0.704365
15	16	0	1.757364	0.014429	-0.769365
16	6	0	2.143981	1.514829	0.184604
17	1	0	1.606636	1.471859	1.129366
18	1	0	1.839161	2.362242	-0.427600
19	1	0	3.222802	1.520070	0.331780
20	8	0	-1.028919	2.000424	1.894729
21	1	0	-0.648501	2.233930	1.040108
22	1	0	-1.523598	1.185955	1.744054

1,2-dmbt H_2O (in water)

Sum of electronic and zero-point Energies= -861.812090 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.852998 (Hartree/particle)
No imaginary frequencies

Standard orientation:



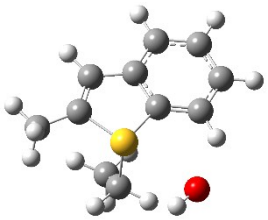
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.507260	1.035859	-0.046184
2	6	0	0.409621	-0.208352	-0.677711
3	6	0	1.497882	-0.943411	-1.107616
4	6	0	2.758562	-0.398020	-0.864485
5	6	0	2.890224	0.840870	-0.234938
6	6	0	1.774618	1.567532	0.175392
7	6	0	-0.793054	1.589000	0.325151
8	6	0	-1.850972	0.837330	0.003685
9	1	0	1.384308	-1.900145	-1.603512
10	1	0	3.641633	-0.944172	-1.173479
11	1	0	3.880498	1.246904	-0.064524
12	1	0	1.884281	2.530281	0.660923
13	1	0	-0.898359	2.537849	0.838890
14	16	0	-1.303299	-0.635034	-0.885596
15	6	0	-1.570973	-1.950949	0.339439
16	1	0	-2.641106	-2.152991	0.351685
17	1	0	-1.209429	-1.611806	1.307271
18	1	0	-1.026697	-2.824637	-0.016485
19	6	0	-3.307970	1.018001	0.232920
20	1	0	-3.712485	0.208850	0.846963
21	1	0	-3.466249	1.961934	0.754661
22	1	0	-3.860353	1.039350	-0.708788
23	8	0	1.299786	-1.108908	2.492037
24	1	0	1.998696	-0.901440	1.860238
25	1	0	0.588560	-0.485337	2.305475

1e2-mbt H_2O (in water)

Sum of electronic and zero-point Energies= -901.086731 (Hartree/particle)
Sum of electronic and thermal Free Energies= -901.129539 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.710803	0.487864	0.286527
2	6	0	-0.945319	-0.355748	-0.525340
3	6	0	-1.310465	-1.647879	-0.852229
4	6	0	-2.510372	-2.116546	-0.317556
5	6	0	-3.298225	-1.297827	0.492265
6	6	0	-2.911494	0.004621	0.798374
7	6	0	-1.088692	1.793698	0.492674
8	6	0	0.091060	1.968155	-0.112192
9	1	0	-0.696427	-2.273500	-1.489595
10	1	0	-2.832257	-3.126392	-0.541205
11	1	0	-4.229996	-1.682683	0.889983
12	1	0	-3.528985	0.636081	1.426715
13	1	0	-1.540413	2.565315	1.105889
14	16	0	0.505494	0.505788	-1.078946
15	6	0	1.875252	-0.261332	-0.105367
16	1	0	2.746294	0.337036	-0.377911
17	1	0	1.978189	-1.247738	-0.561328
18	6	0	1.059469	3.094917	-0.102490
19	1	0	1.216736	3.495753	-1.106194
20	1	0	0.672412	3.888145	0.537232
21	1	0	2.028847	2.773145	0.289991
22	6	0	1.616098	-0.308973	1.381366
23	1	0	2.468858	-0.804935	1.849926
24	1	0	1.530666	0.689452	1.811765
25	1	0	0.720291	-0.884250	1.620657
26	8	0	4.624667	-1.964994	0.256174
27	1	0	3.834992	-2.341727	0.659934
28	1	0	5.346490	-2.562063	0.481687

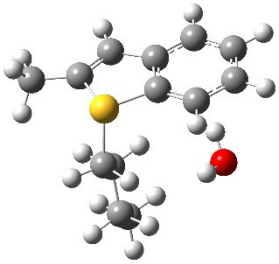


1b2-mbt H_2O (in water)

Sum of electronic and zero-point Energies= -979.637107 (Hartree/particle)
Sum of electronic and thermal Free Energies= -979.681976 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.497510	0.611061	0.754518
2	6	0	-1.220305	0.341162	-0.589902
3	6	0	-1.911449	-0.586906	-1.346716
4	6	0	-2.924811	-1.296000	-0.701976
5	6	0	-3.218960	-1.056504	0.640866
6	6	0	-2.514451	-0.106647	1.377998
7	6	0	-0.636850	1.652181	1.312409
8	6	0	0.255134	2.174577	0.464277
9	1	0	-1.679333	-0.761433	-2.391085
10	1	0	-3.485727	-2.040016	-1.254545



11	1	0	-4.013270	-1.617598	1.119084
12	1	0	-2.752867	0.080226	2.418692
13	1	0	-0.711055	1.981056	2.342829
14	16	0	0.064653	1.426036	-1.163418
15	6	0	1.536608	0.314250	-1.290316
16	1	0	2.313812	0.953073	-1.713189
17	1	0	1.228543	-0.408964	-2.049987
18	6	0	1.304211	3.212405	0.636478
19	1	0	1.111946	4.078042	-0.001282
20	1	0	1.313532	3.536934	1.677155
21	1	0	2.293511	2.818865	0.384905
22	6	0	1.938361	-0.330612	0.019722
23	1	0	2.374676	0.417591	0.686549
24	1	0	1.063362	-0.748637	0.525931
25	8	0	-0.147359	-3.043505	0.203138
26	1	0	0.144231	-2.585833	-0.594864
27	6	0	2.951494	-1.446166	-0.239987
28	1	0	3.819426	-1.035187	-0.765081
29	1	0	2.503801	-2.192071	-0.904940
30	6	0	3.391737	-2.106254	1.061120
31	1	0	2.537717	-2.546309	1.583088
32	1	0	4.116812	-2.901531	0.875768
33	1	0	3.855515	-1.379302	1.733003
34	1	0	-0.609462	-2.376733	0.726615

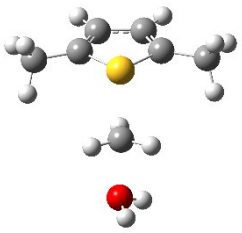
TS neutral hydrolysis (1 H_2O)

TS: 1,2,5-tmt H_2O --> 2,5-dmt + CH_3OH_2 (in water)

Sum of electronic and zero-point Energies= -747.475846 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.512923 (Hartree/particle)
1 imaginary frequency (592.4629i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.951773	1.284049	0.034203
2	6	0	1.595196	0.739955	1.089721
3	6	0	1.609642	-0.705431	1.093960
4	6	0	0.977330	-1.268082	0.041618
5	16	0	0.351672	-0.001338	-1.012136
6	1	0	2.051009	1.344083	1.865219
7	1	0	2.075799	-1.295655	1.873974
8	6	0	-1.800540	-0.029300	-0.164756
9	1	0	-2.027950	-0.943752	-0.691819
10	1	0	-1.394309	-0.067211	0.836547
11	1	0	-2.025113	0.920703	-0.626924
12	6	0	0.695382	2.712471	-0.308826
13	1	0	-0.376454	2.926017	-0.344033
14	1	0	1.146738	3.351827	0.450634
15	1	0	1.120883	2.974946	-1.279789
16	6	0	0.740769	-2.702581	-0.289255
17	1	0	1.205373	-3.329215	0.472796
18	1	0	-0.328358	-2.930875	-0.316265
19	1	0	1.164386	-2.966624	-1.260585
20	8	0	-3.613086	-0.104950	0.628173
21	1	0	-4.257976	0.082377	-0.067174
22	1	0	-3.693402	0.607901	1.276228

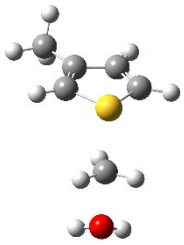


TS: 1,3-dmt H_2O --> 3-mt + CH_3OH_2 (in water)

Sum of electronic and zero-point Energies= -708.194587 (Hartree/particle)
Sum of electronic and thermal Free Energies= -708.230039 (Hartree/particle)
1 imaginary frequency (593.6835i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.929094	0.121594	-1.048976
2	6	0	-1.718983	0.477380	-0.010959
3	6	0	-1.464808	-0.333655	1.168201
4	6	0	-0.509885	-1.266491	0.989871
5	16	0	0.117182	-1.213959	-0.639052
6	1	0	-1.990931	-0.191817	2.104640
7	1	0	-0.116881	-1.989729	1.690158
8	6	0	2.008294	0.015025	-0.145265
9	1	0	2.493784	-0.829663	0.320180
10	1	0	2.193897	0.219562	-1.188471
11	1	0	1.402476	0.687209	0.445265
12	6	0	-2.741646	1.568723	-0.040991
13	1	0	-3.740734	1.157312	0.122646
14	1	0	-2.552518	2.292403	0.755124
15	1	0	-2.734129	2.091091	-0.997360
16	1	0	-0.889940	0.537826	-2.045832
17	8	0	3.626674	1.106765	0.280700
18	1	0	3.420279	2.026274	0.064524
19	1	0	3.763123	1.073294	1.237071

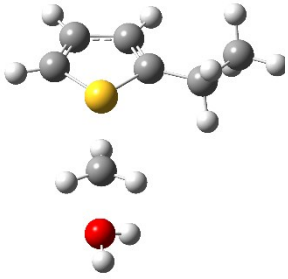


TS: 2e1-mt H_2O --> 2-et + CH_3OH_2 (in water)

Sum of electronic and zero-point Energies= -747.468647 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.505999 (Hartree/particle)
1 imaginary frequency (591.3143i cm-1)

Standard orientation:

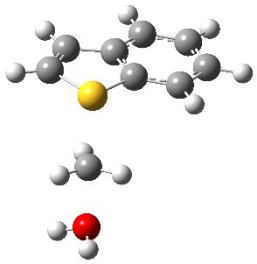
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056661	-0.039364	-0.155746
2	6	0	-1.409895	0.702945	0.917536
3	6	0	-0.694379	1.955011	1.027159
4	6	0	0.199211	2.149145	0.036320
5	16	0	0.183592	0.807190	-1.080375
6	1	0	-2.155598	0.381626	1.634185
7	1	0	-0.855379	2.667179	1.826368
8	6	0	1.954430	-0.354011	-0.168321
9	1	0	2.670776	0.349880	-0.563632
10	1	0	1.539292	-0.205744	0.818755
11	1	0	1.709415	-1.238775	-0.737359
12	6	0	-1.526744	-1.386541	-0.609309
13	1	0	-0.663142	-2.055856	-0.693476
14	1	0	-1.943716	-1.299264	-1.617269
15	8	0	3.473655	-1.316609	0.695799
16	1	0	4.032794	-1.685314	-0.001180
17	1	0	3.111348	-2.068923	1.182910
18	1	0	0.867097	2.980768	-0.136598
19	6	0	-2.560328	-1.988416	0.334618
20	1	0	-3.448871	-1.357082	0.402854



21	1	0	-2.871857	-2.968428	-0.029335
22	1	0	-2.152666	-2.114862	1.339845

TS: 1-mbt H_2O --> bt + CH_3OH_2 (in water)

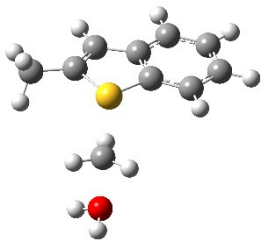
Sum of electronic and zero-point Energies= -822.494907 (Hartree/particle)
Sum of electronic and thermal Free Energies= -822.531958 (Hartree/particle)
1 imaginary frequency (600.0346i cm-1)
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.605569	0.016452	-0.579702
2	6	0	-1.202707	0.700640	0.490130
3	6	0	-0.484323	1.915236	0.833563
4	6	0	0.599552	2.128791	0.069570
5	16	0	0.829113	0.872267	-1.141223
6	1	0	-0.792111	2.582115	1.629282
7	6	0	2.332798	-0.459678	0.009686
8	1	0	3.160601	0.183665	-0.246473
9	1	0	1.772937	-0.291539	0.918836
10	6	0	-1.101507	-1.184936	-1.072554
11	1	0	-0.623666	-1.698546	-1.899036
12	6	0	-2.240105	-1.704193	-0.468048
13	1	0	-2.654128	-2.638783	-0.828074
14	6	0	-2.350260	0.161462	1.079251
15	1	0	-2.829293	0.677083	1.904082
16	6	0	-2.858319	-1.035630	0.595945
17	1	0	-3.746556	-1.461073	1.048198
18	1	0	4.247467	-1.936706	0.452504
19	8	0	3.538286	-1.642099	1.040026
20	1	0	2.093554	-1.301688	-0.623316
21	1	0	1.305549	2.946217	0.106399
22	1	0	3.956195	-1.109088	1.729907

TS: 1,2-dmbt H_2O --> 2-mbt + CH_3OH_2 (in water)

Sum of electronic and zero-point Energies= -861.775740 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.814679 (Hartree/particle)
1 imaginary frequency (604.2843i cm-1)
Standard orientation:



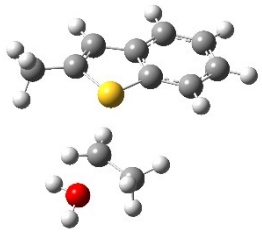
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827401	0.094003	0.580904
2	6	0	-1.194369	-0.754048	-0.475219
3	6	0	-0.168676	-1.736707	-0.774668
4	6	0	0.925714	-1.650929	0.002448
5	16	0	0.768128	-0.335937	1.188861
6	1	0	-0.267866	-2.474029	-1.562935
7	6	0	1.964566	1.250171	-0.011024
8	1	0	2.903530	0.855168	0.347143
9	1	0	1.525898	0.875170	-0.925060
10	6	0	-1.641991	1.124162	1.034153
11	1	0	-1.338529	1.765643	1.853419
12	6	0	-2.867253	1.301757	0.401118

13	1	0	-3.526254	2.096363	0.730669
14	6	0	-2.433054	-0.559985	-1.093469
15	1	0	-2.737161	-1.204344	-1.910823
16	6	0	-3.257543	0.465520	-0.651061
17	1	0	-4.219029	0.621648	-1.126726
18	6	0	2.188112	-2.441630	-0.027661
19	1	0	2.374412	-2.930801	0.931043
20	1	0	2.118263	-3.205790	-0.802217
21	1	0	3.046474	-1.801199	-0.249582
22	1	0	3.477568	3.114437	-0.474829
23	8	0	2.906730	2.613088	-1.072988
24	1	0	3.492157	2.157560	-1.693237
25	1	0	1.478029	2.046582	0.532137

TS: 1e2-mbt H_2O --> 2-mbt + $CH_3CH_2OH_2$ (in water)

Sum of electronic and zero-point Energies= -901.054486 (Hartree/particle)
Sum of electronic and thermal Free Energies= -901.095838 (Hartree/particle)
1 imaginary frequency (552.3564i cm-1)
Standard orientation:

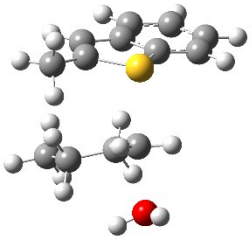
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.001393	-0.074183	-0.561183
2	6	0	-1.403163	0.761972	0.493777
3	6	0	-0.479252	1.858640	0.709518
4	6	0	0.573429	1.866779	-0.129230
5	16	0	0.507992	0.498581	-1.258385
6	1	0	-0.617835	2.608778	1.479478
7	6	0	1.973000	-0.883794	0.117569
8	1	0	2.770304	-0.195552	-0.124735
9	1	0	1.306025	-0.625298	0.929379
10	6	0	-1.734583	-1.190397	-0.950139
11	1	0	-1.415395	-1.815981	-1.775712
12	6	0	-2.901910	-1.472348	-0.249581
13	1	0	-3.494367	-2.335745	-0.529146
14	6	0	-2.583449	0.461430	1.180244
15	1	0	-2.911745	1.096372	1.995746
16	6	0	-3.320970	-0.652881	0.805115
17	1	0	-4.236314	-0.892203	1.334045
18	6	0	1.731973	2.801607	-0.196288
19	1	0	1.818851	3.260749	-1.183452
20	1	0	1.605215	3.590138	0.545931
21	1	0	2.670656	2.279546	0.010917
22	6	0	1.809767	-2.156710	-0.637826
23	1	0	0.766816	-2.473593	-0.660242
24	1	0	2.201631	-2.068236	-1.649944
25	1	0	2.371100	-2.945594	-0.131513
26	1	0	4.012532	-1.920468	1.230219
27	8	0	3.198548	-1.580177	1.625852
28	1	0	3.455576	-0.819493	2.164508



TS: 1b2-mbt H_2O --> 2-mbt + $CH_3CH_2CH_2CH_2OH_2$ (in water)

Sum of electronic and zero-point Energies= -979.604348 (Hartree/particle)
Sum of electronic and thermal Free Energies= -979.648436 (Hartree/particle)
1 imaginary frequency (505.8787i cm-1)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.461714	-0.255936	-0.710195
2	6	0	-1.693699	0.692339	0.300299
3	6	0	-0.777821	1.814726	0.222232
4	6	0	0.102837	1.737530	-0.793893
5	16	0	-0.123608	0.246793	-1.727341
6	1	0	-0.801129	2.649567	0.913335
7	6	0	1.706056	-1.067338	-0.699790
8	1	0	1.266130	-1.924628	-1.191418
9	1	0	2.363747	-0.436155	-1.282947
10	6	0	-2.195402	-1.433889	-0.811996
11	1	0	-1.995994	-2.156544	-1.595180
12	6	0	-3.199602	-1.651157	0.123232
13	1	0	-3.790280	-2.558211	0.069023
14	6	0	-2.712174	0.453362	1.229062
15	1	0	-2.907818	1.174937	2.014580
16	6	0	-3.455941	-0.713509	1.132227
17	1	0	-4.246180	-0.905884	1.848809
18	6	0	1.164789	2.697909	-1.210744
19	1	0	1.272377	3.473983	-0.452002
20	1	0	2.130597	2.202607	-1.339199
21	1	0	0.907821	3.173447	-2.160565
22	6	0	1.482264	-0.832447	0.747543
23	1	0	0.422953	-0.602401	0.916212
24	1	0	1.621534	-1.795900	1.248964
25	6	0	2.364828	0.248385	1.363178
26	1	0	2.317961	1.153732	0.751569
27	1	0	3.407300	-0.084117	1.354784
28	6	0	1.928392	0.565518	2.787799
29	1	0	2.574631	1.319290	3.241662
30	1	0	0.902654	0.946450	2.802750
31	1	0	1.961143	-0.327865	3.417531
32	8	0	3.405021	-2.304677	-0.447050
33	1	0	3.685189	-2.570923	-1.332499
34	1	0	4.128038	-1.775626	-0.085294



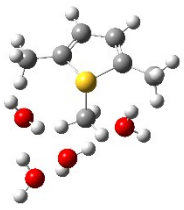
Thiophenium cations + 4 H_2O

1,2,5-tmt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -976.730733 (Hartree/particle)
Sum of electronic and thermal Free Energies= -976.779411 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.145400	0.838251	0.135016
2	6	0	3.113366	-0.082273	0.235508
3	6	0	2.677752	-1.461994	0.062351
4	6	0	1.367760	-1.620027	-0.168251
5	16	0	0.613040	0.003622	-0.294796
6	1	0	4.139972	0.185270	0.456277
7	1	0	3.355206	-2.304585	0.134206



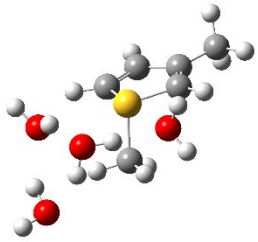
8	6	0	-0.319800	0.108069	1.259515
9	1	0	-1.104872	-0.640042	1.189252
10	1	0	0.362275	-0.092042	2.083310
11	1	0	-0.736950	1.111868	1.306437
12	6	0	2.194815	2.314859	0.306034
13	1	0	1.496619	2.649053	1.077567
14	1	0	3.205554	2.589795	0.610307
15	1	0	1.953045	2.838077	-0.620486
16	6	0	0.562323	-2.854511	-0.364965
17	1	0	1.213495	-3.715633	-0.209269
18	1	0	-0.266068	-2.909456	0.344087
19	1	0	0.148127	-2.905551	-1.373604
20	8	0	-2.114734	-1.395336	-0.893563
21	1	0	-1.969598	-1.905410	-1.697258
22	1	0	-2.394037	-0.497910	-1.154454
23	8	0	-3.000203	1.185686	-0.702770
24	1	0	-3.239019	0.849553	0.177423
25	1	0	-2.217312	1.757056	-0.601255
26	8	0	-3.608462	-0.606154	1.370086
27	1	0	-4.538753	-0.827012	1.487494
28	1	0	-3.256367	-1.225318	0.710708
29	8	0	-0.729400	2.712443	-0.606853
30	1	0	-0.509664	3.354935	0.076796
31	1	0	-0.277589	3.002039	-1.407259

1,3-dmt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -937.449924 (Hartree/particle)
Sum of electronic and thermal Free Energies= -937.495723 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.855150	0.804703	0.059938
2	6	0	2.866511	-0.077592	0.058416
3	6	0	2.410416	-1.462328	-0.138840
4	6	0	1.088893	-1.591707	-0.280243
5	16	0	0.317305	0.002969	-0.278310
6	1	0	3.097704	-2.299997	-0.156542
7	6	0	-0.518379	-0.006761	1.339938
8	1	0	-1.291905	-0.766305	1.274113
9	1	0	0.222467	-0.247086	2.099606
10	1	0	-0.943049	0.983812	1.481235
11	8	0	-2.073451	-1.624617	-0.859765
12	1	0	-2.106703	-2.239668	-1.600176
13	1	0	-2.307424	-0.740695	-1.198262
14	8	0	-2.837067	1.020693	-0.839814
15	1	0	-3.245694	0.710761	-0.013832
16	1	0	-2.131643	1.649789	-0.603425
17	8	0	-3.846921	-0.733265	1.123303
18	1	0	-4.786329	-0.937981	1.062231
19	1	0	-3.387657	-1.350427	0.528525
20	8	0	-0.672661	2.679433	-0.217117
21	1	0	-0.802270	3.250588	0.548734
22	1	0	-0.395162	3.255469	-0.938878
23	1	0	1.866988	1.878777	0.170785
24	1	0	0.474779	-2.465903	-0.437966
25	6	0	4.307611	0.257894	0.245492
26	1	0	4.712003	-0.300925	1.092976
27	1	0	4.878734	-0.034460	-0.639055



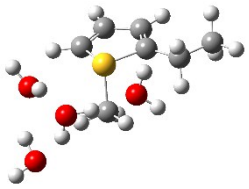
28	1	0	4.447860	1.323541	0.421826

2e1-mt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -976.723946 (Hartree/particle)
Sum of electronic and thermal Free Energies= -976.772215 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.925367	-0.144026	-0.028490
2	6	0	2.518059	-1.346816	0.004576
3	6	0	1.609863	-2.480216	-0.148649
4	6	0	0.323989	-2.138978	-0.283196
5	16	0	0.172923	-0.377395	-0.349729
6	1	0	1.950014	-3.508013	-0.143049
7	6	0	-0.534705	0.041551	1.272046
8	1	0	-1.569321	-0.289718	1.252028
9	1	0	0.041789	-0.472164	2.038832
10	1	0	-0.472138	1.123381	1.368762
11	8	0	-2.624923	-1.294626	-0.753988
12	1	0	-2.720780	-1.896051	-1.500064
13	1	0	-2.676191	-0.382798	-1.097039
14	8	0	-2.801196	1.431106	-0.765170
15	1	0	-3.168766	1.241479	0.114239
16	1	0	-1.953554	1.893930	-0.643165
17	8	0	-3.990505	-0.021071	1.338875
18	1	0	-4.952771	0.015092	1.368292
19	1	0	-3.756824	-0.741359	0.730378
20	8	0	-0.316718	2.631263	-0.630757
21	1	0	0.131818	3.076071	0.097375
22	1	0	0.235664	2.758327	-1.410164
23	1	0	-0.560961	-2.739445	-0.425584
24	1	0	3.583483	-1.472183	0.153468
25	6	0	2.477333	1.233183	0.137571
26	1	0	1.929201	1.740303	0.939849
27	1	0	2.286760	1.807096	-0.774049
28	6	0	3.968469	1.212988	0.450329
29	1	0	4.334908	2.233039	0.570779
30	1	0	4.172596	0.668406	1.374508
31	1	0	4.534788	0.743441	-0.356539

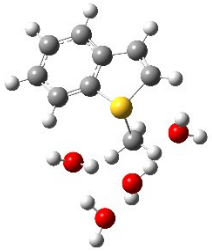


1-mbt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -1051.752516 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1051.800347 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.584658	2.220091	0.117587
2	6	0	1.906989	2.079688	0.230652
3	6	0	2.380289	0.704075	0.087755
4	6	0	1.339435	-0.200326	-0.150263
5	16	0	-0.213677	0.670576	-0.259962
6	6	0	-0.982226	0.221376	1.325520
7	1	0	-1.206132	-0.839931	1.257650



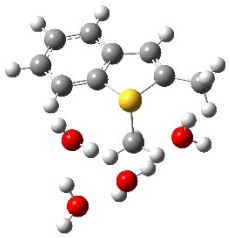
8	1	0	-0.271731	0.434697	2.121305
9	1	0	-1.888217	0.815935	1.415394
10	8	0	-1.621356	-1.882665	-0.920251
11	1	0	-1.430924	-2.389083	-1.717565
12	1	0	-2.291451	-1.210684	-1.153266
13	8	0	-3.617545	-0.019495	-0.742393
14	1	0	-3.775271	-0.471361	0.103039
15	1	0	-3.294621	0.878446	-0.545547
16	8	0	-3.479675	-2.066793	1.199202
17	1	0	-4.169806	-2.737926	1.157579
18	1	0	-2.795214	-2.334590	0.563218
19	8	0	-2.440034	2.457145	-0.335173
20	1	0	-2.736544	3.049344	0.365392
21	1	0	-2.378960	2.991696	-1.135416
22	1	0	2.576118	2.910522	0.419765
23	6	0	1.536634	-1.560643	-0.301688
24	6	0	3.683223	0.222560	0.174060
25	1	0	4.504608	0.906762	0.353124
26	1	0	0.708838	-2.232734	-0.488565
27	6	0	2.847962	-2.024854	-0.201161
28	6	0	3.905073	-1.144170	0.030265
29	1	0	4.915180	-1.530583	0.099372
30	1	0	3.043874	-3.084951	-0.310116
31	1	0	-0.034253	3.102917	0.166570

1,2-dmbt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -1091.032942 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1091.082536 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.705622	2.109751	0.093773
2	6	0	2.016063	1.866475	0.206030
3	6	0	2.410044	0.469841	0.058217
4	6	0	1.323014	-0.376307	-0.183486
5	16	0	-0.176479	0.581703	-0.306081
6	6	0	-0.980051	0.198947	1.277030
7	1	0	-1.355422	-0.818470	1.193073
8	1	0	-0.237717	0.293016	2.067307
9	1	0	-1.797365	0.906201	1.398381
10	8	0	-1.616152	-1.990307	-1.054981
11	1	0	-1.383522	-2.312850	-1.932325
12	1	0	-2.401051	-1.416033	-1.148363
13	8	0	-3.793617	-0.475152	-0.444524
14	1	0	-3.672031	-0.914582	0.412256
15	1	0	-3.479479	0.444118	-0.364416
16	8	0	-2.974581	-2.575716	1.308262
17	1	0	-3.626905	-3.283978	1.344549
18	1	0	-2.439444	-2.731198	0.511476
19	8	0	-2.716854	2.050996	-0.534925
20	1	0	-2.895346	2.750518	0.103996
21	1	0	-2.644303	2.482483	-1.394017
22	1	0	2.731566	2.655293	0.409363
23	6	0	-0.046075	3.386210	0.223189
24	1	0	-0.783841	3.331280	1.027567
25	1	0	0.663187	4.181752	0.454089
26	1	0	-0.571746	3.637078	-0.699673



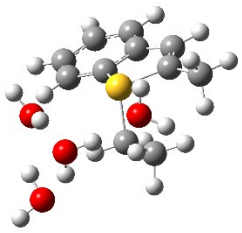
27	6	0	1.446637	-1.745849	-0.331667
28	6	0	3.683752	-0.084211	0.153258
29	1	0	4.540642	0.553138	0.339327
30	1	0	0.584587	-2.371120	-0.522027
31	6	0	2.729122	-2.283222	-0.220867
32	6	0	3.831319	-1.461257	0.013991
33	1	0	4.818569	-1.901582	0.093007
34	1	0	2.866215	-3.353152	-0.323749

1e2-mbt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -1130.310867 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1130.363112 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.693229	2.077179	-0.127950
2	6	0	2.012162	1.867811	-0.049712
3	6	0	2.429257	0.473067	-0.145939
4	6	0	1.351354	-0.403588	-0.308902
5	16	0	-0.165077	0.522010	-0.441052
6	6	0	-1.005521	0.172901	1.163317
7	1	0	-1.281303	-0.876608	1.061374
8	1	0	-1.907922	0.783058	1.118336
9	8	0	-1.538687	-2.106198	-1.124020
10	1	0	-1.208093	-2.441178	-1.964691
11	1	0	-2.311839	-1.540631	-1.312281
12	8	0	-3.754265	-0.572926	-0.731342
13	1	0	-3.675455	-1.002252	0.136559
14	1	0	-3.473643	0.355003	-0.638993
15	8	0	-3.047592	-2.534306	1.191415
16	1	0	-3.697047	-3.243481	1.254803
17	1	0	-2.452681	-2.767726	0.459529
18	8	0	-2.859533	2.026309	-0.766455
19	1	0	-2.925057	2.729100	-0.110258
20	1	0	-2.620079	2.451337	-1.597563
21	1	0	2.717506	2.678046	0.097135
22	6	0	-0.088908	3.335335	-0.002882
23	1	0	-0.816135	3.266738	0.811540
24	1	0	0.599450	4.152830	0.213828
25	1	0	-0.631814	3.565327	-0.921606
26	6	0	1.495587	-1.777798	-0.371495
27	6	0	3.715264	-0.052972	-0.057837
28	1	0	4.564825	0.609263	0.063338
29	1	0	0.640055	-2.429337	-0.488664
30	6	0	2.790214	-2.286070	-0.265527
31	6	0	3.884176	-1.433489	-0.116904
32	1	0	4.881056	-1.852133	-0.041275
33	1	0	2.942815	-3.358113	-0.301792
34	6	0	-0.150330	0.450257	2.377047
35	1	0	-0.718849	0.137789	3.255916
36	1	0	0.780427	-0.119494	2.361392
37	1	0	0.076735	1.511494	2.484119



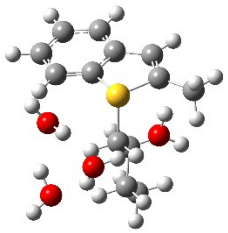
1b2-mbt 4 H_2O (in water)

Sum of electronic and zero-point Energies= -1208.857721 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1208.912445 (Hartree/particle)

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.811469	-1.826958	-1.098681
2	6	0	-2.113047	-1.696347	-0.820122
3	6	0	-2.542999	-0.345969	-0.472506
4	6	0	-1.494720	0.580181	-0.497811
5	16	0	0.001695	-0.218227	-1.041715
6	6	0	1.012387	-0.327621	0.494567
7	1	0	1.311948	0.708069	0.657909
8	1	0	1.884916	-0.903974	0.182558
9	8	0	1.334448	2.539892	-1.022058
10	1	0	1.041166	3.188899	-1.670826
11	1	0	2.095413	2.062930	-1.406515
12	8	0	3.581061	1.009939	-1.263917
13	1	0	3.576551	1.137311	-0.301135
14	1	0	3.308628	0.093881	-1.451247
15	8	0	3.019523	2.282544	1.210150
16	1	0	3.657609	2.964135	1.447398
17	1	0	2.380059	2.696843	0.606470
18	8	0	2.663832	-1.457775	-2.060302
19	1	0	2.771191	-2.331963	-1.668674
20	1	0	2.363180	-1.600205	-2.964805
21	1	0	-2.792872	-2.540950	-0.832252
22	6	0	-0.007313	-3.035612	-1.418240
23	1	0	0.792057	-3.178639	-0.684647
24	1	0	-0.660957	-3.908108	-1.393422
25	1	0	0.448999	-2.963102	-2.407311
26	6	0	-1.651267	1.914601	-0.168869
27	6	0	-3.813015	0.090244	-0.105544
28	1	0	-4.642013	-0.607759	-0.080818
29	1	0	-0.815737	2.601682	-0.198867
30	6	0	-2.928614	2.328660	0.208841
31	6	0	-3.993492	1.428002	0.234965
32	1	0	-4.977450	1.775033	0.528248
33	1	0	-3.091480	3.364678	0.481044
34	6	0	0.295903	-0.930433	1.684707
35	1	0	-0.615801	-0.367444	1.907140
36	1	0	0.007199	-1.963698	1.470997
37	6	0	1.222656	-0.902635	2.902291
38	1	0	1.514893	0.131150	3.111202
39	1	0	2.141229	-1.450647	2.669989
40	6	0	0.550616	-1.510865	4.127410
41	1	0	1.214538	-1.488745	4.994308
42	1	0	-0.358813	-0.963375	4.388724
43	1	0	0.273764	-2.552654	3.944954



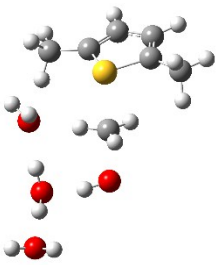
TS neutral hydrolysis (4 H_2O)

TS: 1,2,5-tmt 4 H_2O --> 2,5-dmt + CH_3OH H_3O^+ $2H_2O$ (in water)

Sum of electronic and zero-point Energies= -976.697280 (Hartree/particle)
Sum of electronic and thermal Free Energies= -976.747505 (Hartree/particle)
One imaginary frequency (609.3431i cm-1)

Standard orientation:

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



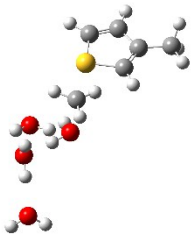
1	6	0	-2.545735	-1.129629	-0.390089
2	6	0	-3.424579	-0.535830	0.445637
3	6	0	-3.096991	0.834691	0.769238
4	6	0	-1.966303	1.287267	0.185096
5	16	0	-1.278393	0.015364	-0.824233
6	1	0	-4.290700	-1.052412	0.841934
7	1	0	-3.696402	1.453048	1.427069
8	6	0	0.335169	-0.673077	0.631685
9	1	0	0.697889	0.340627	0.691259
10	1	0	-0.398859	-1.040591	1.335460
11	1	0	0.764459	-1.346344	-0.094967
12	6	0	-2.503168	-2.526174	-0.912143
13	1	0	-1.598510	-3.043054	-0.579414
14	1	0	-3.368696	-3.076406	-0.541434
15	1	0	-2.518853	-2.549876	-2.003873
16	6	0	-1.291560	2.612742	0.298848
17	1	0	-1.903253	3.273887	0.914042
18	1	0	-0.308080	2.520372	0.769357
19	1	0	-1.151592	3.078575	-0.679392
20	8	0	1.806621	-1.227957	1.874802
21	1	0	1.586724	-0.884477	2.749908
22	1	0	2.530023	-0.656173	1.510045
23	8	0	3.447524	0.434215	0.616742
24	1	0	4.193722	0.027321	0.136694
25	1	0	2.864684	0.852174	-0.042964
26	8	0	5.616374	-0.739030	-0.622952
27	1	0	6.094081	-0.166749	-1.233492
28	1	0	5.446000	-1.558803	-1.100023
29	8	0	1.586815	1.591797	-1.119248
30	1	0	1.538387	1.393681	-2.061107
31	1	0	1.273586	2.497240	-1.015752

TS: 1,3-dmt 4 H_2O --> 3-mt + CH_3OH H_3O^+ $2H_2O$ (in water)

Sum of electronic and zero-point Energies= -937.415789 (Hartree/particle)
Sum of electronic and thermal Free Energies= -937.464738 (Hartree/particle)
One imaginary frequency (605.1735i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281242	0.064291	-1.106345
2	6	0	-3.320873	-0.513177	-0.464530
3	6	0	-3.408906	-0.087105	0.923171
4	6	0	-2.451286	0.787427	1.285345
5	16	0	-1.398023	1.150251	-0.061223
6	1	0	-4.172579	-0.447976	1.601757
7	6	0	0.269283	-0.281302	0.508848
8	1	0	0.602010	0.338472	1.328524
9	1	0	-0.449388	-1.070057	0.679176
10	1	0	0.747660	-0.192659	-0.455016
11	8	0	1.714379	-1.630573	0.979276
12	1	0	1.591512	-1.864543	1.907679
13	1	0	2.532088	-1.068523	0.922786
14	8	0	3.707442	0.069260	0.694549
15	1	0	4.420032	-0.266070	0.117134
16	1	0	3.268447	0.804200	0.224231
17	8	0	5.736470	-0.924654	-0.886960
18	1	0	5.590777	-1.838971	-1.154536
19	1	0	6.589827	-0.909184	-0.439520



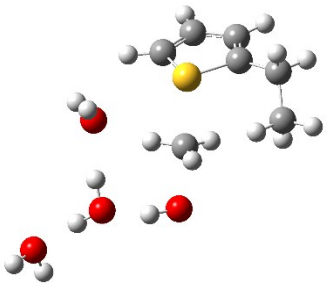
20	8	0	2.295741	2.068072	-0.583904
21	1	0	1.901846	1.699236	-1.382834
22	1	0	2.805256	2.836084	-0.866870
23	1	0	-1.961955	-0.060009	-2.131655
24	1	0	-2.275025	1.257702	2.242270
25	6	0	-4.281669	-1.483210	-1.074856
26	1	0	-4.031915	-1.686760	-2.115854
27	1	0	-4.274706	-2.424828	-0.520872
28	1	0	-5.299629	-1.088513	-1.030318

TS: 2e1-mt 4 H_2O --> 3-et + CH_3OH H_3O^+ $2H_2O$ (in water)

Sum of electronic and zero-point Energies= -976.689772 (Hartree/particle)
Sum of electronic and thermal Free Energies= -976.739310 (Hartree/particle)
One imaginary frequency (610.0777i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.755038	-0.025834	0.033680
2	6	0	3.096359	-0.859511	1.041759
3	6	0	2.176092	-1.957778	1.236328
4	6	0	1.141361	-1.943503	0.372520
5	16	0	1.262266	-0.588150	-0.723714
6	1	0	3.984882	-0.709388	1.643214
7	1	0	2.300376	-2.714625	2.000478
8	6	0	-0.291367	0.720468	0.311018
9	1	0	-0.953702	-0.127916	0.350281
10	1	0	0.361264	0.945110	1.143146
11	1	0	-0.348870	1.400344	-0.525218
12	6	0	3.455886	1.197859	-0.468324
13	1	0	4.302936	1.377869	0.197653
14	1	0	3.869013	0.998874	-1.462143
15	8	0	-1.766250	1.820897	1.158435
16	1	0	-1.868688	1.507452	2.065749
17	1	0	-2.516955	1.444269	0.635000
18	8	0	-3.442510	0.595045	-0.511192
19	1	0	-4.306155	0.275847	-0.187194
20	1	0	-2.935653	-0.178329	-0.818433
21	8	0	-5.901470	-0.209892	0.457035
22	1	0	-6.597916	-0.142243	-0.205982
23	1	0	-6.179952	0.345787	1.193721
24	8	0	-1.716784	-1.468198	-1.338302
25	1	0	-1.570924	-1.599450	-2.281931
26	1	0	-1.770283	-2.348842	-0.949799
27	6	0	2.557644	2.433620	-0.526660
28	1	0	3.141919	3.308079	-0.818023
29	1	0	1.757628	2.317477	-1.262913
30	1	0	2.101433	2.635617	0.445071
31	1	0	0.303426	-2.620273	0.287019

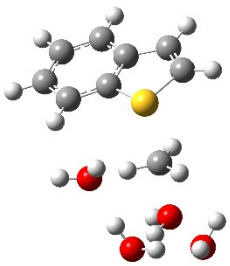


TS: 1-mbt 4 H_2O --> bt + CH_3OH H_3O+ $2H_2O$ (in water)

Sum of electronic and zero-point Energies= -1051.716059 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1051.764432 (Hartree/particle)
One imaginary frequency (618.4700i cm-1)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)



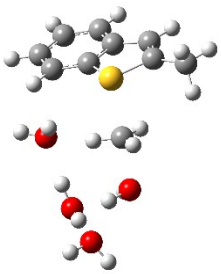
Number	Number	Type	X	Y	Z
1	6	0	1.030791	2.374528	-0.419911
2	6	0	2.232327	2.137416	0.130214
3	6	0	2.589703	0.729351	0.146253
4	6	0	1.594798	-0.077863	-0.426821
5	16	0	0.238064	0.903418	-0.977537
6	6	0	-1.127615	0.435472	0.787344
7	1	0	-1.011427	-0.611739	0.558306
8	1	0	-0.464565	0.925178	1.487063
9	1	0	-1.956246	0.983980	0.363249
10	8	0	-2.349578	-0.075383	2.286867
11	1	0	-1.852666	-0.642109	2.890609
12	1	0	-2.948533	-0.659444	1.757263
13	8	0	-3.747395	-1.363206	0.428505
14	1	0	-4.263001	-0.596496	0.109479
15	1	0	-3.055135	-1.522349	-0.239812
16	8	0	-5.069412	0.926902	-0.326603
17	1	0	-5.516711	0.931627	-1.180116
18	1	0	-4.433272	1.650777	-0.353032
19	8	0	-1.675780	-1.620022	-1.448560
20	1	0	-1.846000	-1.185144	-2.292037
21	1	0	-1.333736	-2.495164	-1.664792
22	1	0	0.526187	3.320205	-0.559074
23	1	0	2.873508	2.915781	0.524968
24	6	0	3.745079	0.123263	0.648392
25	6	0	1.705423	-1.461294	-0.503144
26	1	0	0.924410	-2.065540	-0.949506
27	1	0	4.526604	0.730523	1.091402
28	6	0	2.860958	-2.042387	0.006263
29	6	0	3.871068	-1.256536	0.573865
30	1	0	4.763381	-1.734268	0.961415
31	1	0	2.980294	-3.118518	-0.041188

TS: 12-dmbt 4 H_2O --> 2-mbt + CH_3OH H_3O+ 2H_2O (in water)

Sum of electronic and zero-point Energies= -1090.997751 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1091.049036 (Hartree/particle)
One imaginary frequency (607.7900i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.455434	2.102865	-0.308514
2	6	0	2.574398	1.637543	0.274398
3	6	0	2.713626	0.192737	0.230155
4	6	0	1.636012	-0.427877	-0.421643
5	16	0	0.474293	0.775773	-0.971793
6	6	0	-1.015863	0.578066	0.748113
7	1	0	-1.083968	-0.477982	0.539706
8	1	0	-0.298897	0.955730	1.464296
9	1	0	-1.714654	1.257723	0.283286
10	8	0	-2.355693	0.344711	2.209391
11	1	0	-1.937718	-0.195368	2.891985
12	1	0	-2.994880	-0.239684	1.724640
13	8	0	-3.796514	-1.167093	0.581146
14	1	0	-4.576930	-0.705021	0.218978
15	1	0	-3.169476	-1.297624	-0.155085
16	8	0	-6.007999	0.157812	-0.410601
17	1	0	-6.533077	0.576928	0.280559
18	1	0	-6.607304	-0.433076	-0.880293

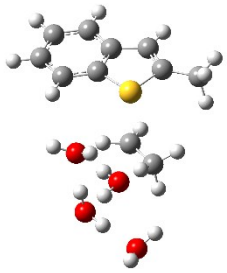


19	8	0	-1.844835	-1.490261	-1.396764
20	1	0	-2.007806	-1.021271	-2.223151
21	1	0	-1.616535	-2.393858	-1.644028
22	1	0	3.303551	2.288655	0.742675
23	6	0	3.739476	-0.606136	0.742268
24	6	0	1.546068	-1.805315	-0.576824
25	1	0	0.706126	-2.260533	-1.087874
26	1	0	4.582153	-0.146663	1.246855
27	6	0	2.576605	-2.580450	-0.055763
28	6	0	3.662167	-1.984844	0.596065
29	1	0	4.454174	-2.610489	0.991204
30	1	0	2.536994	-3.658362	-0.161091
31	6	0	0.941959	3.496355	-0.426545
32	1	0	0.784556	3.776002	-1.470554
33	1	0	-0.013106	3.605102	0.095468
34	1	0	1.659144	4.188411	0.015473

TS: 1e2-mbt 4 H_2O --> 2-mbt + CH_3CH_2OH H_3O+ 2H_2O (in water)

Sum of electronic and zero-point Energies= -1130.276108 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1130.326784 (Hartree/particle)
One imaginary frequency (568.6345i cm-1)

Standard orientation:



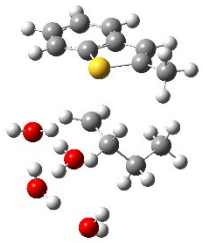
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.486176	2.122752	-0.188002
2	6	0	2.576484	1.636636	0.434020
3	6	0	2.751582	0.203665	0.294731
4	6	0	1.736155	-0.384343	-0.477136
5	16	0	0.585510	0.833130	-1.013847
6	6	0	-1.047743	0.412164	0.680304
7	1	0	-0.925733	-0.621934	0.398060
8	1	0	-0.366537	0.831880	1.409407
9	8	0	-2.109335	-0.364330	2.289480
10	1	0	-1.498172	-0.937024	2.769788
11	1	0	-2.703938	-0.953021	1.761400
12	8	0	-3.547487	-1.688852	0.468966
13	1	0	-4.245975	-1.047963	0.231914
14	1	0	-2.917359	-1.697036	-0.275699
15	8	0	-5.479409	0.186781	-0.143467
16	1	0	-6.087200	-0.055395	-0.851193
17	1	0	-5.053079	1.004665	-0.423527
18	8	0	-1.658889	-1.552085	-1.598409
19	1	0	-1.929842	-0.949930	-2.301027
20	1	0	-1.376453	-2.364429	-2.034153
21	1	0	3.257046	2.265282	0.996637
22	6	0	3.758562	-0.612519	0.818759
23	6	0	1.690277	-1.749899	-0.735262
24	1	0	0.899508	-2.182935	-1.336221
25	1	0	4.552933	-0.176309	1.414380
26	6	0	2.699220	-2.542528	-0.199711
27	6	0	3.723641	-1.977463	0.568909
28	1	0	4.500033	-2.616563	0.973513
29	1	0	2.691664	-3.610293	-0.384838
30	6	0	0.962098	3.518289	-0.227138
31	1	0	0.747564	3.839392	-1.248563
32	1	0	0.039011	3.605463	0.352761
33	1	0	1.700388	4.195483	0.203562

34	6	0	-2.158636	1.232904	0.110592
35	1	0	-2.526645	0.808385	-0.823005
36	1	0	-2.983323	1.256803	0.826225
37	1	0	-1.847987	2.265330	-0.050841

TS: 1b2-mbt 4 H_2O --> 2-mbt + $CH_3CH_2CH_2CH_2OH$ H_3O+ 2H_2O (in water)

Sum of electronic and zero-point Energies= -1208.820409 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1208.873723 (Hartree/particle)
One imaginary frequency (510.5460i cm-1)

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.542496	1.854074	0.812942
2	6	0	-2.518006	1.687893	-0.099804
3	6	0	-2.896414	0.305452	-0.326736
4	6	0	-2.163335	-0.584972	0.473467
5	16	0	-0.992748	0.289342	1.451768
6	6	0	0.732925	-0.207534	-0.115488
7	1	0	0.737579	-1.195852	0.322476
8	1	0	-0.003527	-0.000932	-0.880951
9	8	0	1.761282	-1.192519	-1.717781
10	1	0	1.145393	-1.892801	-1.966953
11	1	0	2.501028	-1.625769	-1.226103
12	8	0	3.717613	-2.140201	-0.148180
13	1	0	4.314596	-1.368537	-0.187050
14	1	0	3.239199	-2.084256	0.701442
15	8	0	5.236066	0.172661	-0.482288
16	1	0	4.885487	0.843661	0.115735
17	1	0	4.988135	0.460777	-1.368996
18	8	0	2.166004	-1.958015	2.146195
19	1	0	2.205016	-1.076007	2.534839
20	1	0	2.398870	-2.572260	2.851915
21	1	0	-2.993475	2.522156	-0.602867
22	6	0	-3.852951	-0.213194	-1.204882
23	6	0	-2.328463	-1.963226	0.409795
24	1	0	-1.742654	-2.630600	1.032004
25	1	0	-4.436799	0.455427	-1.827825
26	6	0	-3.283620	-2.456335	-0.472657
27	6	0	-4.039412	-1.587503	-1.268505
28	1	0	-4.778593	-1.995988	-1.948069
29	1	0	-3.444834	-3.525907	-0.539610
30	6	0	-0.972496	3.113515	1.373478
31	1	0	-1.313388	3.260440	2.401791
32	1	0	0.119390	3.107049	1.386040
33	1	0	-1.307451	3.961191	0.774480
34	6	0	1.839633	0.756159	0.184203
35	1	0	2.697104	0.185491	0.548462
36	1	0	1.538272	1.391515	1.021550
37	6	0	2.248447	1.654435	-0.989718
38	1	0	3.000303	2.351646	-0.608764
39	1	0	2.740797	1.047880	-1.751574
40	6	0	1.098246	2.435683	-1.616088
41	1	0	1.473392	3.105028	-2.393302
42	1	0	0.362477	1.777286	-2.085099
43	1	0	0.577580	3.047795	-0.875481

Hydrolysis products

2,5-dmt (in water)

Sum of electronic and zero-point Energies= -631.452714 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.484190 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.259504	-0.125911	-0.000010
2	6	0	0.716218	-1.374690	0.000065
3	6	0	-0.716218	-1.374690	-0.000079
4	6	0	-1.259504	-0.125911	-0.000007
5	16	0	0.000000	1.075324	0.000045
6	1	0	1.322821	-2.273039	0.000098
7	1	0	-1.322820	-2.273039	-0.000135
8	6	0	-2.702981	0.265567	-0.000004
9	1	0	-2.962647	0.856446	0.881596
10	1	0	-2.962614	0.856537	-0.881552
11	1	0	-3.322941	-0.632335	-0.000064
12	6	0	2.702980	0.265567	-0.000049
13	1	0	2.962619	0.856468	-0.881643
14	1	0	2.962642	0.856515	0.881506
15	1	0	3.322941	-0.632334	-0.000031

3-mt (in water)

Sum of electronic and zero-point Energies= -592.175366 (Hartree/particle)
Sum of electronic and thermal Free Energies= -592.204137 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035790	1.147308	0.000273
2	6	0	-0.321641	1.244781	-0.000034
3	6	0	-0.979779	-0.030634	0.000093
4	6	0	-0.080577	-1.056672	0.000049
5	16	0	1.553454	-0.497266	-0.000291
6	1	0	-0.851915	2.189778	-0.000039
7	1	0	-0.285335	-2.118428	0.000059
8	1	0	1.766090	1.944012	0.000437
9	6	0	-2.470647	-0.197015	0.000200
10	1	0	-2.917011	0.272912	0.880076
11	1	0	-2.917192	0.273143	-0.879460
12	1	0	-2.748778	-1.251779	0.000099

2-et (in water)

Sum of electronic and zero-point Energies= -631.448575 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.480981 (Hartree/particle)
No imaginary frequencies

Standard orientation:

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

1	6	0	2.017731	-0.431991	0.177085
2	6	0	1.917587	0.923905	0.229765
3	6	0	0.584058	1.384307	-0.007883
4	6	0	-0.307433	0.376851	-0.238255
5	16	0	0.491383	-1.165133	-0.160502
6	1	0	2.757988	1.575954	0.431954
7	1	0	0.293610	2.428460	-0.009788
8	6	0	-1.780051	0.480733	-0.503952
9	1	0	-2.013476	0.051634	-1.483134
10	1	0	-2.027333	1.543894	-0.557716
11	6	0	-2.633270	-0.199344	0.568030
12	1	0	-3.695459	-0.050341	0.363493
13	1	0	-2.448149	-1.275776	0.599928
14	1	0	-2.414466	0.210952	1.556623
15	1	0	2.893420	-1.049413	0.317936

bt (in water)

Sum of electronic and zero-point Energies= -706.473085 (Hartree/particle)
Sum of electronic and thermal Free Energies= -706.504076 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.109155	0.847460	0.000054
2	6	0	-0.062213	-0.551174	-0.000044
3	6	0	1.028000	-1.425751	0.000051
4	6	0	2.301728	-0.882192	0.000256
5	6	0	2.492565	0.510655	0.000357
6	6	0	1.411480	1.373248	0.000257
7	6	0	-1.152918	1.545510	-0.000074
8	6	0	-2.211035	0.704829	-0.000249
9	1	0	0.880734	-2.499879	-0.000023
10	1	0	3.162625	-1.541148	0.000337
11	1	0	3.500568	0.909566	0.000521
12	1	0	1.558863	2.448007	0.000335
13	1	0	-1.242435	2.624621	-0.000029
14	1	0	-3.261297	0.961890	-0.000363
15	16	0	-1.756227	-0.977410	-0.000276

2-mbt (in water)

Sum of electronic and zero-point Energies= -745.762621 (Hartree/particle)
Sum of electronic and thermal Free Energies= -745.796033 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.399704	0.792853	-0.000101
2	6	0	-0.427481	-0.615580	-0.000053
3	6	0	-1.628615	-1.327121	-0.000167
4	6	0	-2.815826	-0.610946	-0.000318
5	6	0	-2.808461	0.793174	-0.000361
6	6	0	-1.614902	1.494708	-0.000257

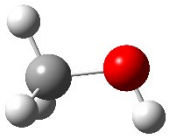
7	6	0	0.948531	1.305382	0.000047
8	6	0	1.895966	0.338631	0.000216
9	1	0	-1.634627	-2.411612	-0.000132
10	1	0	-3.760074	-1.143956	-0.000406
11	1	0	-3.749306	1.332280	-0.000478
12	1	0	-1.610726	2.579824	-0.000289
13	1	0	1.187134	2.362975	0.000041
14	16	0	1.192259	-1.270802	0.000183
15	6	0	3.381845	0.494853	0.000453
16	1	0	3.830796	0.031793	0.882630
17	1	0	3.831151	0.031379	-0.881323
18	1	0	3.641395	1.554434	0.000266

CH_3OH (in water)

Sum of electronic and zero-point Energies= -115.652133 (Hartree/particle)
Sum of electronic and thermal Free Energies= -115.674944 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.047801	0.667548	0.000000
2	1	0	-1.088100	0.989019	0.000000
3	1	0	0.446192	1.062694	0.890998
4	1	0	0.446192	1.062694	-0.890998
5	8	0	-0.047801	-0.756886	0.000000
6	1	0	0.864928	-1.064603	0.000000

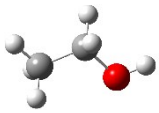


CH_3CH_2OH (in water)

Sum of electronic and zero-point Energies= -154.930260 (Hartree/particle)
Sum of electronic and thermal Free Energies= -154.955708 (Hartree/particle)
No imaginary frequencies

Standard orientation:

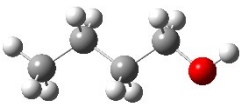
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.220728	-0.222314	0.000066
2	1	0	1.294113	-0.855567	-0.887195
3	1	0	1.294082	-0.855333	0.887494
4	1	0	2.068480	0.465948	-0.000025
5	6	0	-0.078091	0.547950	-0.000062
6	1	0	-0.147745	1.186545	0.886322
7	1	0	-0.147584	1.186503	-0.886498
8	8	0	-1.153304	-0.395486	-0.000140
9	1	0	-1.990732	0.081978	0.001001



$CH_3CH_2CH_2CH_2OH$ (in water)

Sum of electronic and zero-point Energies= -233.475235 (Hartree/particle)
Sum of electronic and thermal Free Energies= -233.505399 (Hartree/particle)
No imaginary frequencies

Standard orientation:



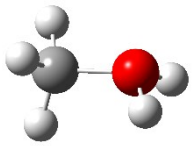
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.502679	-0.291587	-0.000095
2	1	0	2.553825	-0.935162	-0.882917
3	1	0	2.554314	-0.934692	0.883040
4	1	0	3.390335	0.345444	-0.000516
5	6	0	1.219712	0.532013	0.000042
6	1	0	1.202899	1.186913	0.877921
7	1	0	1.202705	1.186813	-0.877903
8	6	0	-0.026947	-0.348926	0.000177
9	1	0	-0.021168	-0.999401	0.882065
10	1	0	-0.021126	-0.999719	-0.881477
11	6	0	-1.298545	0.470832	-0.000017
12	1	0	-1.335684	1.113537	-0.886755
13	1	0	-1.335865	1.113663	0.886621
14	8	0	-2.417719	-0.418994	-0.000073
15	1	0	-3.229888	0.100565	-0.000140

CH_3OH_2 (in water)

Sum of electronic and zero-point Energies= -116.049316 (Hartree/particle)
Sum of electronic and thermal Free Energies= -116.072427 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001269	0.771656	0.000000
2	1	0	-1.042928	1.063234	0.000000
3	1	0	0.508882	1.095918	0.902214
4	1	0	0.508882	1.095918	-0.902214
5	8	0	0.001269	-0.687304	0.000000
6	1	0	0.828452	-1.189729	0.000000
7	1	0	-0.821059	-1.196848	0.000000

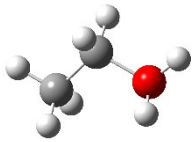


$CH_3CH_2OH_2$ (in water)

Sum of electronic and zero-point Energies= -155.332001 (Hartree/particle)
Sum of electronic and thermal Free Energies= -155.357600 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.266384	-0.257787	0.029597
2	1	0	1.297703	-0.984464	-0.784122
3	1	0	1.317092	-0.777689	0.986365
4	1	0	2.139093	0.391222	-0.059769
5	6	0	0.038206	0.599031	-0.058399
6	1	0	-0.063978	1.296381	0.767889
7	1	0	-0.075069	1.107849	-1.012249
8	8	0	-1.153097	-0.290453	0.093186
9	1	0	-1.992319	0.201527	0.142519
10	1	0	-1.225286	-0.958667	-0.613306

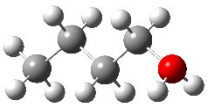


$CH_3CH_2CH_2CH_2OH_2$ (in water)

Sum of electronic and zero-point Energies= -233.877073 (Hartree/particle)
Sum of electronic and thermal Free Energies= -233.907118 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.549608	-0.331708	0.002580
2	1	0	-2.590964	-0.939080	0.910574
3	1	0	-2.575493	-1.009643	-0.854590
4	1	0	-3.451324	0.283451	-0.029444
5	6	0	-1.292183	0.529054	-0.019865
6	1	0	-1.286152	1.155750	-0.917051
7	1	0	-1.291753	1.206861	0.839540
8	6	0	-0.026555	-0.328013	0.005826
9	1	0	0.004946	-0.972455	-0.878066
10	1	0	-0.027267	-0.971030	0.891502
11	6	0	1.194468	0.553843	0.029623
12	1	0	1.292017	1.138867	0.940546
13	1	0	1.284650	1.196326	-0.842985
14	8	0	2.450002	-0.250974	-0.005363
15	1	0	2.515484	-0.896214	0.723025
16	1	0	2.569106	-0.724098	-0.849129

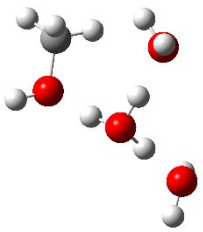


$CH_3OH\ H_3O+\ 2H_2O$ (in water)

Sum of electronic and zero-point Energies= -345.295283 (Hartree/particle)
Sum of electronic and thermal Free Energies= -345.331809 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.258293	-0.481433	0.461615
2	1	0	2.513676	0.353132	-0.194045
3	1	0	3.165007	-0.999538	0.774140
4	1	0	1.730891	-0.113632	1.340038
5	8	0	1.371842	-1.393533	-0.200713
6	1	0	1.805263	-1.756072	-0.982423
7	1	0	0.096674	-0.597178	-0.573094
8	8	0	-0.661221	0.053399	-0.755638
9	1	0	-1.506411	-0.253194	-0.289304
10	1	0	-0.384989	0.966190	-0.411776
11	8	0	-2.838408	-0.682626	0.390235
12	1	0	-3.354621	-1.277331	-0.166582
13	1	0	-2.704105	-1.138403	1.229560
14	8	0	0.117585	2.330230	0.137111
15	1	0	0.156012	3.012581	-0.543880
16	1	0	1.014463	2.232282	0.479723

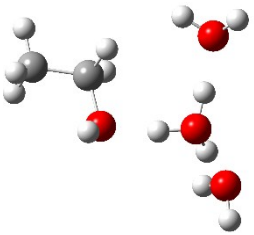


$CH3CH_2OH\ H_3O+\ 2H_2O$ (in water)

Sum of electronic and zero-point Energies= -384.573377 (Hartree/particle)
Sum of electronic and thermal Free Energies= -384.611441 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)



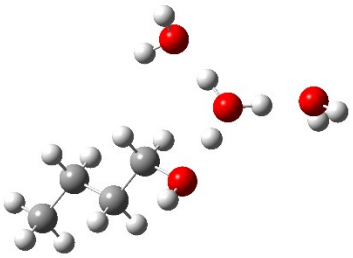
Number	Number	Type	X	Y	Z
1	6	0	-1.756493	0.035489	-0.148641
2	1	0	-1.768266	0.961840	0.432322
3	1	0	-1.164568	0.201200	-1.049694
4	8	0	-1.041133	-0.972734	0.591913
5	1	0	-1.490563	-1.133589	1.431778
6	1	0	0.405803	-0.443175	0.778577
7	8	0	1.300829	0.035647	0.800786
8	1	0	1.980797	-0.470033	0.244440
9	1	0	1.164155	0.961672	0.415556
10	8	0	3.073012	-1.208782	-0.574371
11	1	0	3.464187	-1.948218	-0.094221
12	1	0	2.734228	-1.566539	-1.403551
13	8	0	0.873114	2.363231	-0.219285
14	1	0	1.130416	3.096485	0.352109
15	1	0	-0.067008	2.474740	-0.406079
16	6	0	-3.158439	-0.417848	-0.483118
17	1	0	-3.727745	-0.614692	0.428770
18	1	0	-3.677003	0.362418	-1.044352
19	1	0	-3.141413	-1.326852	-1.087436

$CH3CH_2CH_2CH_2OH\ H_3O+\ 2H_2O$ (in water)

Sum of electronic and zero-point Energies= -463.119009 (Hartree/particle)
Sum of electronic and thermal Free Energies= -463.161613 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.674432	-0.124954	-0.235626
2	1	0	0.608393	0.797080	-0.822218
3	1	0	0.292925	0.075463	0.767379
4	8	0	-0.224787	-1.101950	-0.794337
5	1	0	0.045704	-1.304598	-1.699351
6	1	0	-1.633001	-0.481621	-0.766514
7	8	0	-2.502022	0.042988	-0.692299
8	1	0	-3.123633	-0.404189	-0.029656
9	1	0	-2.273536	0.978459	-0.379868
10	8	0	-4.111777	-1.072678	0.970829
11	1	0	-4.757108	-1.635616	0.527082
12	1	0	-3.658347	-1.629318	1.614807
13	8	0	-1.815888	2.388778	0.111454
14	1	0	-2.157130	3.111474	-0.428439
15	1	0	-0.853623	2.460133	0.092262
16	6	0	2.099696	-0.635476	-0.190516
17	1	0	2.418866	-0.887261	-1.208821
18	1	0	2.131412	-1.558881	0.397249
19	6	0	3.051534	0.397558	0.406886
20	1	0	2.720981	0.652736	1.419253
21	1	0	3.001815	1.320884	-0.179951
22	6	0	4.489394	-0.108091	0.446814
23	1	0	4.849709	-0.341757	-0.558780
24	1	0	5.164721	0.634369	0.877883
25	1	0	4.567301	-1.018690	1.047153

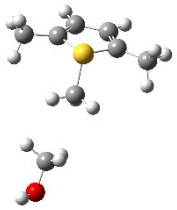


Methanolysis S_N2

Thiophenium cations + nucleophile

1,2,5-tmt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -786.765605 (Hartree/particle)
Sum of electronic and thermal Free Energies= -786.807220 (Hartree/particle)
No imaginary frequencies

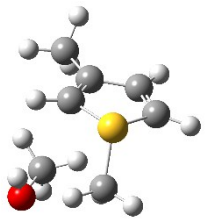


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311822	1.407476	0.104486
2	6	0	-1.992856	0.993680	1.181067
3	6	0	-2.262073	-0.440201	1.235868
4	6	0	-1.792815	-1.150366	0.201639
5	16	0	-1.053855	-0.008367	-0.964624
6	1	0	-2.306203	1.677413	1.961385
7	1	0	-2.787384	-0.906566	2.061206
8	6	0	0.723564	-0.336379	-0.755132
9	1	0	0.948886	-0.336503	0.309614
10	1	0	0.920928	-1.303183	-1.216148
11	1	0	1.252164	0.450557	-1.291072
12	6	0	-1.819489	-2.603409	-0.111605
13	1	0	-2.368576	-2.804111	-1.034384
14	1	0	-0.807933	-3.003787	-0.223680
15	1	0	-2.309762	-3.130221	0.707868
16	6	0	-0.825419	2.745900	-0.322695
17	1	0	0.256262	2.744107	-0.482766
18	1	0	-1.305974	3.064992	-1.250490
19	1	0	-1.057382	3.469972	0.459144
20	6	0	3.894081	-0.184036	0.302997
21	1	0	3.438389	-0.603663	1.199456
22	1	0	3.584844	-0.774040	-0.564832
23	1	0	3.554884	0.848838	0.181842
24	8	0	5.303793	-0.246640	0.486232
25	1	0	5.739172	0.117183	-0.292772

1,3-dmt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -747.483802 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.521582 (Hartree/particle)
No imaginary frequencies



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.334574	0.357608	-1.060739
2	6	0	-0.251329	1.414350	-0.237675
3	6	0	-1.098386	1.274578	0.957872
4	6	0	-1.806940	0.144963	1.007214
5	16	0	-1.541220	-0.791262	-0.474137
6	1	0	-1.130095	2.030390	1.734590
7	1	0	-2.502190	-0.231386	1.744587
8	6	0	-0.564400	-2.205869	0.126197
9	1	0	-1.256153	-2.852409	0.664555
10	1	0	-0.177330	-2.717078	-0.753759
11	1	0	0.229042	-1.835797	0.771202
12	6	0	0.610801	2.610719	-0.449323

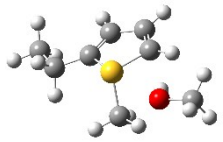
13	1	0	-0.008366	3.510501	-0.501350
14	1	0	1.288323	2.733764	0.400209
15	1	0	1.193674	2.527737	-1.365825
16	1	0	0.138959	0.174398	-2.015886
17	8	0	2.686068	-1.331566	-0.115914
18	1	0	2.081822	-1.235777	-0.861080
19	6	0	2.661535	-0.142464	0.665240
20	1	0	3.446972	-0.237550	1.414881
21	1	0	2.864464	0.739301	0.051439
22	1	0	1.701610	-0.016689	1.177231

2e1- mt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -786.760023 (Hartree/particle)
Sum of electronic and thermal Free Energies= -786.800311 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.209362	0.079542	-0.241376
2	6	0	-0.686614	-0.597213	-1.273728
3	6	0	0.536880	-0.023709	-1.828698
4	6	0	0.961295	1.082839	-1.209069
5	16	0	-0.224807	1.557780	0.014923
6	1	0	-1.121648	-1.513324	-1.654378
7	1	0	1.065087	-0.470438	-2.662293
8	1	0	1.809028	1.725244	-1.401271
9	6	0	-2.388234	-0.169530	0.639676
10	1	0	-2.045242	-0.217864	1.679703
11	1	0	-3.070637	0.684167	0.579628
12	6	0	-3.116024	-1.456506	0.269403
13	1	0	-3.960397	-1.606128	0.943865
14	1	0	-3.500743	-1.414383	-0.751702
15	1	0	-2.457847	-2.323935	0.355754
16	6	0	0.582002	1.228179	1.611240
17	1	0	1.387732	1.953797	1.712142
18	1	0	-0.172895	1.400615	2.377296
19	1	0	0.941132	0.201565	1.612173
20	8	0	1.916206	-1.606796	0.732418
21	1	0	1.880406	-2.521260	0.429324
22	6	0	3.162947	-1.036324	0.350178
23	1	0	3.304112	-1.069377	-0.733777
24	1	0	3.154753	0.006089	0.671718
25	1	0	3.997078	-1.548562	0.837953

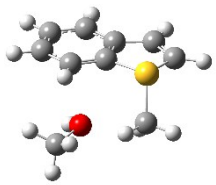


1-mbt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -861.788835 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.828273 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.173394	-1.321882	-0.417880
2	6	0	-0.258876	-0.438519	0.662786
3	6	0	0.794253	-0.151524	1.508504



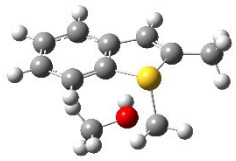
4	6	0	2.004990	-0.788957	1.237430
5	6	0	2.121467	-1.680500	0.171044
6	6	0	1.039263	-1.958625	-0.660946
7	6	0	-1.419619	-1.405372	-1.177328
8	6	0	-2.399336	-0.621622	-0.721824
9	1	0	0.694907	0.539135	2.338188
10	1	0	2.862738	-0.586994	1.868849
11	1	0	3.072608	-2.167414	-0.012483
12	1	0	1.135047	-2.653276	-1.487858
13	1	0	-1.534381	-2.043060	-2.046179
14	1	0	-3.412445	-0.487613	-1.074095
15	16	0	-1.900728	0.245668	0.753813
16	6	0	-1.645950	1.947961	0.163707
17	1	0	-1.025504	1.920211	-0.729787
18	1	0	-1.172773	2.489837	0.981474
19	1	0	-2.634811	2.360003	-0.036384
20	8	0	1.410960	1.489922	-1.382834
21	1	0	2.090200	1.098001	-1.943434
22	6	0	2.026072	2.386275	-0.465993
23	1	0	2.505376	3.220153	-0.987399
24	1	0	1.240883	2.781275	0.179609
25	1	0	2.768904	1.876255	0.154162

1,2-dmbt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -901.073635 (Hartree/particle)
Sum of electronic and thermal Free Energies= -901.114881 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.516756	0.817140	0.777541
2	6	0	0.423667	0.655119	-0.608414
3	6	0	1.515506	0.621272	-1.455320
4	6	0	2.773633	0.735011	-0.864443
5	6	0	2.900036	0.896844	0.515499
6	6	0	1.781692	0.939788	1.345273
7	6	0	-0.785749	0.812623	1.439137
8	6	0	-1.841433	0.671552	0.630943
9	1	0	1.404387	0.511250	-2.528202
10	1	0	3.658625	0.706148	-1.489287
11	1	0	3.888384	0.993219	0.950661
12	1	0	1.888218	1.069822	2.416551
13	1	0	-0.894243	0.899777	2.514793
14	16	0	-1.287739	0.620073	-1.086558
15	6	0	-1.596828	-1.105881	-1.561379
16	1	0	-2.664909	-1.183485	-1.763160
17	1	0	-1.285048	-1.756180	-0.746892
18	1	0	-1.034001	-1.283236	-2.477414
19	6	0	-3.299171	0.573174	0.902962
20	1	0	-3.701711	-0.378701	0.544710
21	1	0	-3.461762	0.632255	1.979749
22	1	0	-3.852449	1.381499	0.418909
23	8	0	0.018032	-2.421411	0.950402
24	1	0	0.226350	-2.351324	1.889332
25	6	0	1.226499	-2.594317	0.217756
26	1	0	1.698515	-3.551456	0.458381
27	1	0	0.967926	-2.588693	-0.841773
28	1	0	1.933641	-1.784728	0.418036

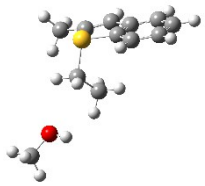


1e2-mbt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -940.347709 (Hartree/particle)
Sum of electronic and thermal Free Energies= -940.393184 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.193181	0.338838	0.343293
2	6	0	-1.395573	-0.400935	-0.536006
3	6	0	-1.657586	-1.709823	-0.894683
4	6	0	-2.779745	-2.306999	-0.320770
5	6	0	-3.596557	-1.593950	0.557191
6	6	0	-3.317268	-0.271341	0.892246
7	6	0	-1.687060	1.690738	0.568882
8	6	0	-0.559529	1.996004	-0.081569
9	1	0	-1.023266	-2.252810	-1.586166
10	1	0	-3.018525	-3.335025	-0.567462
11	1	0	-4.466751	-2.078025	0.985788
12	1	0	-3.958383	0.278699	1.571955
13	1	0	-2.180530	2.396690	1.228036
14	16	0	-0.054100	0.609150	-1.115944
15	6	0	1.430556	-0.042332	-0.225986
16	1	0	2.190793	0.714518	-0.427015
17	1	0	1.684754	-0.942477	-0.788062
18	6	0	0.288525	3.216313	-0.081476
19	1	0	0.371269	3.647416	-1.082030
20	1	0	-0.154755	3.956398	0.585587
21	1	0	1.298652	2.992446	0.274922
22	6	0	1.202678	-0.291044	1.245628
23	1	0	2.139988	-0.665848	1.663038
24	1	0	0.940333	0.623174	1.780240
25	1	0	0.432362	-1.044643	1.416963
26	8	0	4.382162	-0.829815	0.263441
27	1	0	3.944876	-1.676354	0.412211
28	6	0	5.787533	-1.040505	0.172886
29	1	0	6.248827	-0.064948	0.022467
30	1	0	6.183105	-1.480616	1.092326
31	1	0	6.038809	-1.686260	-0.673032

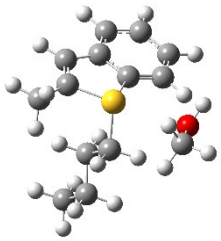


1b2-mbt CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -1018.900739 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1018.947451 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.763454	-0.939372	0.622670
2	6	0	-1.243194	0.175265	-0.045793
3	6	0	-1.768173	0.672007	-1.224304
4	6	0	-2.876607	0.010301	-1.751725
5	6	0	-3.426593	-1.093256	-1.099751
6	6	0	-2.879695	-1.575755	0.086576
7	6	0	-0.999575	-1.293099	1.816344



8	6	0	0.056480	-0.511508	2.066950
9	1	0	-1.332839	1.527455	-1.724450
10	1	0	-3.313352	0.363978	-2.678499
11	1	0	-4.292654	-1.586817	-1.526160
12	1	0	-3.307526	-2.437712	0.586321
13	1	0	-1.258148	-2.138343	2.444864
14	16	0	0.133068	0.831118	0.871510
15	6	0	1.608515	0.395735	-0.147765
16	1	0	2.451642	0.706831	0.473859
17	1	0	1.525147	1.078056	-0.995760
18	6	0	1.095739	-0.565744	3.129030
19	1	0	1.101486	0.346065	3.731208
20	1	0	0.895911	-1.415930	3.782011
21	1	0	2.093100	-0.688335	2.695265
22	6	0	1.680258	-1.061529	-0.555330
23	1	0	1.723203	-1.700530	0.331456
24	1	0	0.785659	-1.338166	-1.121922
25	8	0	0.189204	3.123878	-0.875975
26	6	0	2.924477	-1.298939	-1.413616
27	1	0	3.815104	-0.998296	-0.852172
28	1	0	2.881629	-0.662414	-2.303193
29	6	0	3.044092	-2.761176	-1.827986
30	1	0	2.173923	-3.077170	-2.410220
31	1	0	3.933460	-2.926428	-2.440555
32	1	0	3.115464	-3.413626	-0.953183
33	1	0	-0.658912	3.580840	-0.824870
34	6	0	1.167305	3.889403	-0.178928
35	1	0	2.114222	3.354150	-0.256753
36	1	0	1.286952	4.878464	-0.628766
37	1	0	0.906357	4.005021	0.876931

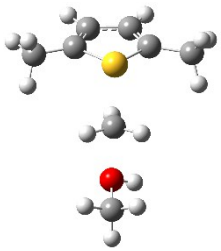
Transition state methanolisys S_N2

TS: 1,2,5-tmt CH_3OH --> 2,5-dmt + CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -786.738664 (Hartree/particle)
Sum of electronic and thermal Free Energies= -786.777881 (Hartree/particle)
1 imaginary frequency (589.2981i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.409723	1.269678	0.005366
2	6	0	2.087293	0.720133	1.035638
3	6	0	2.076402	-0.725631	1.050041
4	6	0	1.390181	-1.285192	0.030936
5	16	0	0.738853	-0.013120	-1.004102
6	1	0	2.586174	1.319763	1.788186
7	1	0	2.567782	-1.317596	1.813533
8	6	0	-1.349489	0.020816	-0.060469
9	1	0	-1.610300	-0.932465	-0.498786
10	1	0	-0.900175	0.060253	0.922641
11	1	0	-1.610614	0.930668	-0.583012
12	6	0	1.158904	2.700299	-0.332191
13	1	0	0.089281	2.929770	-0.319135
14	1	0	1.652763	3.336388	0.403739
15	1	0	1.543455	2.954875	-1.322544
16	6	0	1.126841	-2.718549	-0.284548
17	1	0	1.604855	-3.347050	0.468187



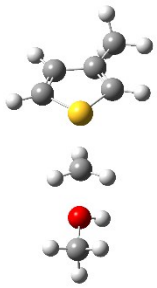
18	1	0	0.055036	-2.936955	-0.281813
19	1	0	1.521340	-2.993780	-1.265502
20	8	0	-3.120902	0.024263	0.830702
21	1	0	-3.189250	0.852108	1.326350
22	6	0	-4.196572	-0.068407	-0.111234
23	1	0	-4.100762	-1.034020	-0.604216
24	1	0	-5.147756	-0.020066	0.419157
25	1	0	-4.135968	0.735049	-0.848008

TS: 1,3-dmt CH_3OH --> 3-mt + CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -747.456906 (Hartree/particle)
Sum of electronic and thermal Free Energies= -747.495329 (Hartree/particle)
1 imaginary frequency (597.8013i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.427681	0.180615	-1.044313
2	6	0	2.226603	0.513157	-0.005883
3	6	0	2.009939	-0.348728	1.145463
4	6	0	1.072379	-1.294191	0.947411
5	16	0	0.416607	-1.193549	-0.669230
6	1	0	2.550024	-0.232322	2.077849
7	6	0	-1.494169	-0.066018	-0.103501
8	1	0	-1.912868	-0.933162	0.386926
9	1	0	-0.912141	0.646594	0.464601
10	1	0	-1.738968	0.130224	-1.137887
11	8	0	-3.127633	0.935128	0.467491
12	1	0	-3.068381	1.823185	0.089731
13	6	0	-4.328747	0.295235	0.019492
14	1	0	-4.389561	-0.659118	0.539324
15	1	0	-5.189819	0.909477	0.283764
16	1	0	-4.300480	0.132629	-1.059764
17	1	0	1.361224	0.634860	-2.023416
18	1	0	0.706630	-2.052942	1.624983
19	6	0	3.220837	1.631037	-0.006423
20	1	0	3.197847	2.181335	-0.947121
21	1	0	3.013395	2.326022	0.811054
22	1	0	4.231334	1.242338	0.144234

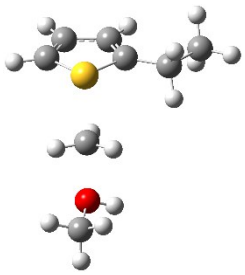


TS: 2e1-mt CH_3OH --> 2-et + CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -786.731455 (Hartree/particle)
Sum of electronic and thermal Free Energies= -786.771204 (Hartree/particle)
1 imaginary frequency (589.5102i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.472652	0.202843	-0.160983
2	6	0	2.025117	-0.486668	0.862208
3	6	0	1.580729	-1.860248	0.954611
4	6	0	0.690029	-2.200775	0.001870
5	16	0	0.381253	-0.851528	-1.063452
6	1	0	1.926846	-2.548706	1.715607
7	6	0	-1.537845	-0.107533	-0.071080
8	1	0	-2.084323	-0.988058	-0.376568

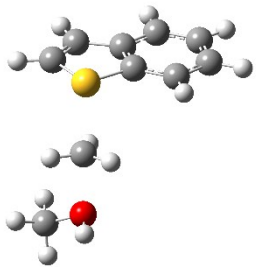


9	1	0	-1.043011	-0.087992	0.890560
10	1	0	-1.562612	0.776954	-0.692371
11	8	0	-3.200491	0.499266	0.845263
12	1	0	-3.023978	1.370943	1.225726
13	6	0	-4.304060	0.580927	-0.065530
14	1	0	-4.472718	-0.424352	-0.447227
15	1	0	-5.191283	0.923590	0.467485
16	1	0	-4.075002	1.259156	-0.889808
17	1	0	0.194857	-3.145593	-0.172722
18	1	0	2.730754	-0.047938	1.556983
19	6	0	1.628367	1.633271	-0.575995
20	1	0	1.961806	1.671796	-1.617907
21	1	0	0.644908	2.117618	-0.552660
22	6	0	2.602793	2.397532	0.312249
23	1	0	2.672612	3.434429	-0.020994
24	1	0	2.274396	2.399884	1.354126
25	1	0	3.603931	1.962501	0.268809

TS: 1-mbt CH_3OH --> bt + CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -861.758173 (Hartree/particle)
Sum of electronic and thermal Free Energies= -861.796827 (Hartree/particle)
1 imaginary frequency (594.0098i cm-1)

Standard orientation:



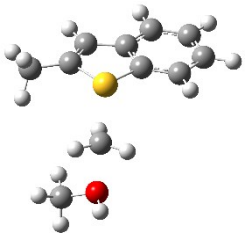
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089294	0.051417	-0.576176
2	6	0	-1.543830	0.591165	0.636763
3	6	0	-0.846605	1.816855	0.987585
4	6	0	0.085319	2.177351	0.090611
5	16	0	0.183052	1.057814	-1.265495
6	1	0	-1.059979	2.384475	1.885417
7	6	0	1.956702	-0.202717	-0.531043
8	1	0	2.665838	0.574753	-0.779317
9	1	0	1.515966	-0.246623	0.455621
10	6	0	-1.596919	-1.127340	-1.109631
11	1	0	-1.233723	-1.527029	-2.049943
12	6	0	-2.597501	-1.775772	-0.395331
13	1	0	-3.016066	-2.697080	-0.784408
14	6	0	-2.555049	-0.075589	1.335058
15	1	0	-2.924563	0.327915	2.271643
16	6	0	-3.072840	-1.252552	0.813261
17	1	0	-3.858281	-1.775285	1.347611
18	1	0	3.958013	-1.638402	-0.565680
19	8	0	3.420791	-1.329154	0.177123
20	1	0	1.741418	-0.978232	-1.252543
21	6	0	4.239950	-0.610956	1.108216
22	1	0	3.576620	-0.229420	1.882638
23	1	0	4.967800	-1.291293	1.550865
24	1	0	4.751031	0.216514	0.613196
25	1	0	0.741171	3.036757	0.099960

TS: 1,2-dmbt CH_3OH --> 2-mbt + CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -901.040141 (Hartree/particle)
Sum of electronic and thermal Free Energies= -901.081543 (Hartree/particle)
1 imaginary frequency (598.4449i cm-1)

Standard orientation:

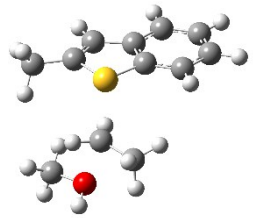
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.219831	-0.103148	-0.582154
2	6	0	-1.571324	0.519555	0.625303
3	6	0	-0.708068	1.645067	0.937593
4	6	0	0.253844	1.877466	0.027009
5	16	0	0.160023	0.709847	-1.313052
6	1	0	-0.819630	2.245516	1.833543
7	6	0	1.796852	-0.704870	-0.533497
8	1	0	2.577640	-0.039645	-0.875215
9	1	0	1.393177	-0.612643	0.465886
10	6	0	-1.893726	-1.210320	-1.081935
11	1	0	-1.604711	-1.672649	-2.019484
12	6	0	-2.958634	-1.704312	-0.336704
13	1	0	-3.506208	-2.567688	-0.697389
14	6	0	-2.648358	0.008521	1.354818
15	1	0	-2.941104	0.475864	2.288966
16	6	0	-3.330964	-1.098340	0.868536
17	1	0	-4.167139	-1.500476	1.429659
18	6	0	1.342839	2.894295	0.021137
19	1	0	1.330316	3.493204	-0.892277
20	1	0	1.221055	3.561803	0.875075
21	1	0	2.325218	2.417856	0.096591
22	1	0	3.664296	-2.279869	-0.536561
23	8	0	3.155787	-1.923833	0.205605
24	1	0	1.458676	-1.503005	-1.179256
25	6	0	4.029904	-1.247418	1.118361
26	1	0	3.405155	-0.848094	1.915270
27	1	0	4.742760	-1.960337	1.533032
28	1	0	4.558631	-0.435691	0.615361



TS: 1e2-mbt CH_3OH --> 2-mbt + $CH_3CH_2OHCH_3$ (in methanol)

Sum of electronic and zero-point Energies= -940.319478 (Hartree/particle)
Sum of electronic and thermal Free Energies= -940.362521 (Hartree/particle)
1 imaginary frequency (542.4199i cm-1)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378571	-0.066491	-0.522731
2	6	0	-1.590224	0.758649	0.594287
3	6	0	-0.625170	1.839956	0.668228
4	6	0	0.274980	1.848545	-0.332924
5	16	0	0.003947	0.493882	-1.451301
6	1	0	-0.622622	2.579463	1.461473
7	6	0	1.675790	-0.856787	-0.360355
8	1	0	2.416927	-0.206654	-0.805489
9	1	0	1.201602	-0.541448	0.560258
10	6	0	-2.181496	-1.165550	-0.806601
11	1	0	-2.006458	-1.779517	-1.683069
12	6	0	-3.224142	-1.445458	0.069061
13	1	0	-3.868699	-2.295373	-0.124876
14	6	0	-2.648782	0.460308	1.457949
15	1	0	-2.835083	1.085604	2.324644
16	6	0	-3.453481	-0.638794	1.189823
17	1	0	-4.276196	-0.874496	1.855761
18	6	0	1.426168	2.763499	-0.576811
19	1	0	1.343018	3.259845	-1.546705

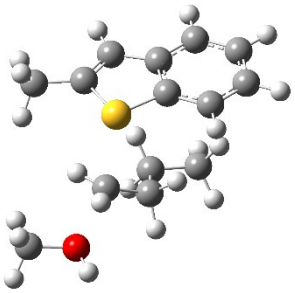


20	1	0	1.456050	3.526133	0.202510
21	1	0	2.374048	2.216764	-0.560558
22	6	0	1.350141	-2.174642	-0.973534
23	1	0	0.330407	-2.481246	-0.738961
24	1	0	1.504380	-2.162341	-2.051981
25	1	0	2.016217	-2.933714	-0.554211
26	1	0	3.880154	-1.872523	0.396527
27	8	0	3.182420	-1.444174	0.911914
28	6	0	3.716580	-0.296728	1.580311
29	1	0	2.884156	0.194842	2.082606
30	1	0	4.452358	-0.612776	2.320676
31	1	0	4.176462	0.389676	0.866683

TS: 1b2-mbt CH_3OH --> 2-mbt + $CH_3CH_2CH_2CH_2OHCH_3$ (in methanol)

Sum of electronic and zero-point Energies= -1018.869183 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1018.915097 (Hartree/particle)
1 imaginary frequency (495.9264i cm-1)

Standard orientation:



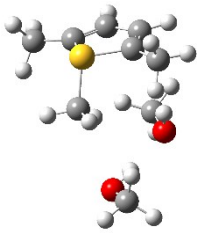
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.421991	0.369334	0.755480
2	6	0	1.932470	0.817960	-0.474921
3	6	0	1.086940	1.825416	-1.087574
4	6	0	-0.016348	2.127536	-0.378685
5	16	0	-0.081902	1.194107	1.134521
6	1	0	1.317742	2.296715	-2.036245
7	6	0	-1.893587	-0.366777	0.617462
8	1	0	-2.292541	-0.195889	1.609058
9	1	0	-2.159729	0.335532	-0.161140
10	6	0	2.066120	-0.591393	1.526864
11	1	0	1.662646	-0.913864	2.480412
12	6	0	3.254137	-1.124122	1.036830
13	1	0	3.778050	-1.876771	1.614939
14	6	0	3.125878	0.266459	-0.948030
15	1	0	3.537560	0.597135	-1.895489
16	6	0	3.775494	-0.700136	-0.190033
17	1	0	4.702094	-1.130811	-0.552759
18	6	0	-1.102694	3.104423	-0.674536
19	1	0	-1.143526	3.889624	0.084433
20	1	0	-0.918045	3.569650	-1.643534
21	1	0	-2.084211	2.623090	-0.706274
22	6	0	-1.113823	-1.592776	0.305630
23	1	0	-0.293281	-1.697237	1.022731
24	1	0	-1.765042	-2.447804	0.520070
25	1	0	-4.068808	-1.714940	0.868732
26	8	0	-3.792979	-1.174152	0.115928
27	6	0	-4.740238	-0.123724	-0.095437
28	1	0	-4.451533	0.384167	-1.014337
29	1	0	-5.741316	-0.540561	-0.212853
30	1	0	-4.729585	0.584442	0.736544
31	6	0	-0.606360	-1.632941	-1.133075
32	1	0	-0.182559	-0.659730	-1.398682
33	1	0	-1.456814	-1.792515	-1.803554
34	6	0	0.442987	-2.717789	-1.333688
35	1	0	0.047616	-3.704096	-1.073873
36	1	0	0.779531	-2.755720	-2.372119
37	1	0	1.318206	-2.531753	-0.703552

Methanolisys S_N3

Thiophenium cations + nucleophile

1,2,5-tmt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -902.427796 (Hartree/particle)
Sum of electronic and thermal Free Energies= -902.469732 (Hartree/particle)
No imaginary frequencies

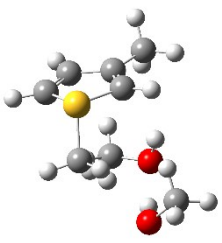


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.068052	1.371693	-0.576331
2	6	0	1.581240	1.455957	0.659100
3	6	0	2.162789	0.220507	1.176865
4	6	0	2.103719	-0.829893	0.348247
5	16	0	1.387480	-0.276974	-1.198449
6	1	0	1.555401	2.376208	1.231345
7	1	0	2.590563	0.146683	2.170133
8	6	0	-0.264022	-1.040191	-1.173393
9	1	0	-0.127845	-2.099779	-1.387693
10	1	0	-0.703931	-0.879127	-0.192159
11	1	0	-0.838825	-0.568834	-1.969579
12	6	0	0.393656	2.367258	-1.451849
13	1	0	-0.587977	2.012529	-1.778953
14	1	0	0.257532	3.293626	-0.892530
15	1	0	0.988003	2.582057	-2.343300
16	6	0	2.522098	-2.248514	0.496141
17	1	0	2.961422	-2.384453	1.485117
18	1	0	1.666917	-2.923898	0.402769
19	1	0	3.261522	-2.529520	-0.257299
20	8	0	-3.279946	-1.200570	0.126894
21	1	0	-2.845134	-0.528740	0.681806
22	8	0	-1.936106	0.904758	1.335611
23	1	0	-1.369191	1.301733	0.662829
24	6	0	-3.844338	-0.526242	-0.987737
25	1	0	-4.218510	-1.279519	-1.681453
26	1	0	-4.677935	0.115901	-0.685363
27	1	0	-3.099885	0.087465	-1.505949
28	6	0	-1.132678	0.426444	2.413516
29	1	0	-0.516399	1.226490	2.830523
30	1	0	-1.817528	0.068921	3.181906
31	1	0	-0.492558	-0.401786	2.095642

1,3-dmt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -863.143794 (Hartree/particle)
Sum of electronic and thermal Free Energies= -863.187222 (Hartree/particle)
No imaginary frequencies



Standard orientation:

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

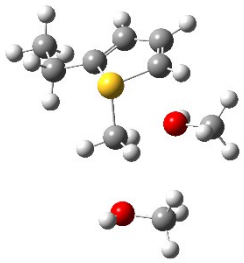
1	6	0	0.961742	-0.301148	-1.171906
2	6	0	1.617498	0.748665	-0.648674
3	6	0	2.218394	0.450669	0.661128
4	6	0	2.025239	-0.798797	1.088954
5	16	0	1.185012	-1.732630	-0.159678
6	1	0	2.761059	1.197808	1.229026
7	6	0	-0.454206	-2.057295	0.563270
8	1	0	-0.290756	-2.731414	1.403055
9	1	0	-0.896815	-1.115173	0.877163
10	1	0	-1.043163	-2.550776	-0.208348
11	8	0	-3.266899	-0.288859	0.296832
12	1	0	-2.806030	0.549524	0.475338
13	8	0	-1.528437	1.862339	0.293773
14	1	0	-0.983919	1.512699	-0.422889
15	6	0	-3.089776	-0.575965	-1.082067
16	1	0	-3.512779	-1.562102	-1.275306
17	1	0	-3.605589	0.157382	-1.710319
18	1	0	-2.029600	-0.587973	-1.359168
19	6	0	-0.769999	1.912708	1.501320
20	1	0	0.132439	2.516599	1.377273
21	1	0	-1.406632	2.379428	2.252277
22	1	0	-0.494010	0.911931	1.844323
23	1	0	2.344177	-1.299865	1.992233
24	1	0	0.456567	-0.405730	-2.122233
25	6	0	1.733676	2.093878	-1.282353
26	1	0	1.361971	2.862972	-0.599850
27	1	0	2.784526	2.318783	-1.483761
28	1	0	1.175655	2.143856	-2.216844

2e1-mt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -902.416479 (Hartree/particle)
Sum of electronic and thermal Free Energies= -902.463408 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.847115	-0.251291	-0.053695
2	6	0	2.017116	0.847076	0.695922
3	6	0	1.401676	2.058365	0.158171
4	6	0	0.745306	1.881430	-0.993675
5	16	0	0.970021	0.217465	-1.547113
6	1	0	2.552318	0.836735	1.637613
7	1	0	1.461487	3.016906	0.659218
8	1	0	0.218423	2.581765	-1.626041
9	6	0	2.250569	-1.676305	0.132247
10	1	0	1.349770	-2.300940	0.122116
11	1	0	2.855924	-1.992123	-0.723275
12	6	0	3.018255	-1.886673	1.431750
13	1	0	3.289158	-2.938701	1.531777
14	1	0	3.937443	-1.296980	1.448569
15	1	0	2.414279	-1.609756	2.298648
16	6	0	-0.650533	-0.579569	-1.296691
17	1	0	-1.322683	-0.164131	-2.046172
18	1	0	-0.493521	-1.642030	-1.479299
19	1	0	-0.974702	-0.377063	-0.278233
20	8	0	-1.366044	0.743835	1.518385
21	1	0	-1.354394	0.765163	2.482282

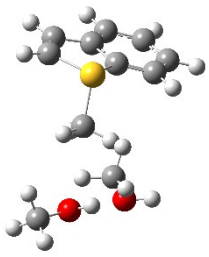


22	6	0	-2.011597	1.914440	1.031814
23	1	0	-1.483105	2.819647	1.345038
24	1	0	-2.000534	1.863107	-0.057702
25	1	0	-3.048652	1.968969	1.375280
26	8	0	-3.100458	-1.993831	0.012521
27	1	0	-3.013174	-2.324155	-0.888970
28	6	0	-3.915851	-0.827581	0.002970
29	1	0	-4.903955	-1.038853	-0.415792
30	1	0	-4.032663	-0.507678	1.037832
31	1	0	-3.452082	-0.018701	-0.569208

1-mbt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -977.446012 (Hartree/particle)
Sum of electronic and thermal Free Energies= -977.493711 (Hartree/particle)
No imaginary frequencies

Standard orientation:



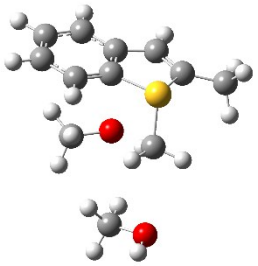
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.715482	-0.274011	-0.373634
2	6	0	-2.621311	0.657750	0.144001
3	6	0	-2.214991	2.039341	-0.109934
4	6	0	-1.063643	2.164698	-0.773267
5	16	0	-0.392179	0.571731	-1.211153
6	1	0	-2.797862	2.891913	0.218829
7	6	0	0.993399	0.384173	-0.037716
8	1	0	1.792014	1.035556	-0.390583
9	1	0	0.640337	0.667640	0.951007
10	6	0	-1.869969	-1.642195	-0.257266
11	1	0	-1.155209	-2.340353	-0.678279
12	6	0	-2.996752	-2.089000	0.432293
13	1	0	-3.156782	-3.154123	0.552729
14	6	0	-3.744661	0.189956	0.818926
15	1	0	-4.466082	0.889348	1.226292
16	6	0	-3.919399	-1.184256	0.959032
17	1	0	-4.790439	-1.558897	1.484489
18	1	0	3.284394	-0.626689	1.171776
19	8	0	3.224181	0.018377	1.898262
20	1	0	1.294964	-0.661369	-0.081567
21	6	0	4.133523	1.071620	1.617290
22	1	0	4.174035	1.719354	2.493600
23	1	0	5.139889	0.688687	1.421082
24	1	0	3.807151	1.670051	0.759668
25	1	0	-0.530931	3.047681	-1.097712
26	8	0	3.712660	-1.518217	-0.336865
27	1	0	3.471786	-2.440113	-0.484167
28	6	0	3.789806	-0.828999	-1.581587
29	1	0	2.836115	-0.861394	-2.115660
30	1	0	4.043104	0.207110	-1.358561
31	1	0	4.570532	-1.257826	-2.214505

1,2-dmbt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -1016.731059 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1016.780349 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.842578	0.281793	0.374248
2	6	0	1.198078	0.090456	-0.852033
3	6	0	1.436069	-0.984379	-1.688029
4	6	0	2.356824	-1.933420	-1.244949
5	6	0	3.010596	-1.775237	-0.022507
6	6	0	2.765678	-0.672279	0.792269
7	6	0	1.401886	1.490584	1.065757
8	6	0	0.465427	2.204988	0.433947
9	1	0	0.929438	-1.095014	-2.639883
10	1	0	2.567289	-2.798298	-1.862947
11	1	0	3.724825	-2.524816	0.298805
12	1	0	3.280773	-0.554491	1.739033
13	1	0	1.788216	1.780765	2.036607
14	16	0	0.091103	1.446204	-1.161352
15	6	0	-1.553035	0.720157	-0.855227
16	1	0	-1.533473	0.232510	0.117763
17	1	0	-1.741643	0.026148	-1.672945
18	1	0	-2.264048	1.544376	-0.889421
19	8	0	-0.753129	-0.886392	1.955352
20	1	0	-0.832796	-1.019477	2.907347
21	6	0	-0.503892	-2.138665	1.327020
22	1	0	-1.306536	-2.853536	1.532012
23	1	0	-0.457507	-1.959387	0.252534
24	1	0	0.446537	-2.566777	1.657866
25	6	0	-0.273144	3.437829	0.811375
26	1	0	-1.348508	3.246904	0.870223
27	1	0	0.071321	3.772415	1.790353
28	1	0	-0.109473	4.240310	0.088540
29	6	0	-3.653057	-1.603972	0.075518
30	1	0	-3.177842	-1.266709	0.995541
31	1	0	-2.890993	-2.010896	-0.595683
32	1	0	-4.371367	-2.392625	0.316891
33	8	0	-4.300908	-0.475530	-0.500984
34	1	0	-4.763615	-0.752395	-1.300295

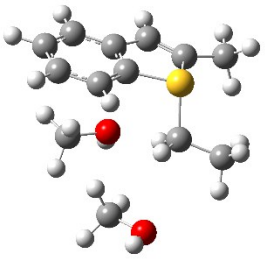


1e2-mbt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -1056.006147 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1056.056026 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.989210	0.153390	0.075548
2	6	0	1.051933	-0.019781	-0.947213
3	6	0	0.969730	-1.155618	-1.731057
4	6	0	1.882536	-2.174971	-1.458840
5	6	0	2.832923	-2.029888	-0.447250
6	6	0	2.897129	-0.871895	0.323925
7	6	0	1.839131	1.429396	0.767623
8	6	0	0.838571	2.206697	0.337777
9	1	0	0.233922	-1.255473	-2.521220
10	1	0	1.852921	-3.085236	-2.046174
11	1	0	3.534842	-2.834232	-0.258362



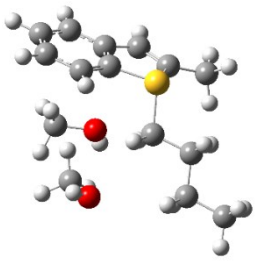
12	1	0	3.636327	-0.766106	1.110251
13	1	0	2.484163	1.727360	1.586963
14	16	0	0.033269	1.430698	-1.079493
15	6	0	-1.583161	0.807997	-0.432186
16	1	0	-1.369402	0.436498	0.570579
17	1	0	-1.805994	-0.023561	-1.103037
18	8	0	-0.338891	-0.643951	2.301320
19	1	0	-0.509578	-0.594658	3.249060
20	6	0	0.009293	-1.981573	1.961017
21	1	0	-0.785147	-2.682102	2.236530
22	1	0	0.150455	-2.016321	0.880872
23	1	0	0.938640	-2.285376	2.451445
24	6	0	0.372522	3.541687	0.802079
25	1	0	-0.590111	3.467062	1.313709
26	1	0	1.102821	3.941850	1.506663
27	1	0	0.264901	4.243787	-0.027479
28	6	0	-2.914704	-2.103586	0.337343
29	1	0	-2.682244	-1.431910	1.163104
30	1	0	-2.002932	-2.301385	-0.235034
31	1	0	-3.290095	-3.046601	0.745230
32	8	0	-3.899453	-1.458331	-0.462490
33	1	0	-4.180356	-2.058600	-1.162374
34	6	0	-2.650144	1.880620	-0.489991
35	1	0	-3.585473	1.427662	-0.152752
36	1	0	-2.432727	2.722149	0.167362
37	1	0	-2.800290	2.247430	-1.506749

1b2-mbt 2CH_3OH (in methanol)

Sum of electronic and zero-point Energies= -1134.555205 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1134.609199 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.244830	0.972706	-0.028459
2	6	0	1.409643	0.320344	-0.940756
3	6	0	1.772352	-0.818538	-1.635822
4	6	0	3.045764	-1.330084	-1.385062
5	6	0	3.905477	-0.695830	-0.487213
6	6	0	3.517360	0.454426	0.195262
7	6	0	1.611136	2.134796	0.585160
8	6	0	0.356447	2.384938	0.193438
9	1	0	1.105312	-1.293639	-2.346400
10	1	0	3.369132	-2.224860	-1.904067
11	1	0	4.893770	-1.108168	-0.317297
12	1	0	4.188364	0.940108	0.895104
13	1	0	2.113303	2.750370	1.323561
14	16	0	-0.112508	1.223716	-1.106946
15	6	0	-1.370411	0.105201	-0.355858
16	1	0	-1.035476	-0.083512	0.665408
17	1	0	-1.279983	-0.805787	-0.953505
18	8	0	0.488641	-0.525875	2.283958
19	1	0	0.186697	-0.399679	3.191119
20	6	0	1.484883	-1.541786	2.263120
21	1	0	1.096322	-2.489565	2.648296
22	1	0	1.788752	-1.680190	1.226039
23	1	0	2.360792	-1.250373	2.850458



24	6	0	-0.603450	3.439790	0.618982
25	1	0	-1.399339	3.018692	1.238552
26	1	0	-0.067451	4.182596	1.211478
27	1	0	-1.063163	3.940663	-0.235459
28	6	0	-0.783455	-3.104369	0.403182
29	1	0	-1.197827	-2.501038	1.210797
30	1	0	0.075439	-2.583020	-0.029537
31	1	0	-0.452713	-4.064844	0.808627
32	8	0	-1.815875	-3.282277	-0.561237
33	1	0	-1.494051	-3.858578	-1.263812
34	6	0	-2.761543	0.707043	-0.465740
35	1	0	-2.821458	1.649282	0.084986
36	1	0	-2.993649	0.921202	-1.513729
37	6	0	-3.789477	-0.276603	0.096711
38	1	0	-3.732822	-1.216047	-0.461563
39	1	0	-3.538056	-0.510119	1.136704
40	6	0	-5.203081	0.288957	0.020330
41	1	0	-5.481656	0.511338	-1.013670
42	1	0	-5.933019	-0.420092	0.417883
43	1	0	-5.288063	1.215083	0.595739

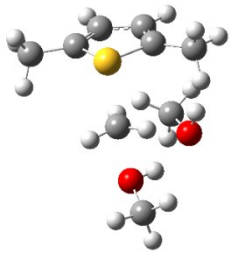
Transition state methanolysis S_N3

TS: 1,2,5-tmt $2CH_3OH$ --> 2,5-dmt + $CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -902.401098 (Hartree/particle)
Sum of electronic and thermal Free Energies= -902.446299 (Hartree/particle)
1 imaginary frequency (598.5068i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.214328	1.065477	0.933837
2	6	0	-1.600759	1.519595	-0.276727
3	6	0	-2.085649	0.490117	-1.170775
4	6	0	-2.067206	-0.754146	-0.647831
5	16	0	-1.434225	-0.688231	0.999850
6	1	0	-1.548825	2.568236	-0.547041
7	1	0	-2.426365	0.689988	-2.180195
8	6	0	0.714033	-1.049655	0.394540
9	1	0	0.655660	-2.129711	0.393348
10	1	0	0.516120	-0.503023	-0.515551
11	1	0	1.092674	-0.549284	1.275587
12	6	0	-0.651920	1.794979	2.106685
13	1	0	0.334042	1.412324	2.388631
14	1	0	-0.550542	2.852808	1.859655
15	1	0	-1.301262	1.705472	2.981183
16	6	0	-2.436267	-2.064392	-1.255782
17	1	0	-2.777910	-1.903712	-2.279270
18	1	0	-1.579537	-2.744322	-1.282332
19	1	0	-3.236129	-2.557206	-0.698227
20	8	0	2.607456	-1.134620	-0.289450
21	1	0	2.732100	-0.169897	-0.419118
22	8	0	2.228237	1.544779	-0.565036
23	1	0	1.598326	1.763909	0.133625
24	6	0	3.535550	-1.635764	0.672603
25	1	0	3.296673	-2.684877	0.840586
26	1	0	4.551467	-1.552598	0.282779
27	1	0	3.456733	-1.085693	1.613684



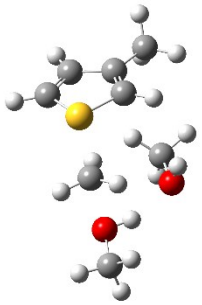
28	6	0	1.633189	1.803062	-1.837859
29	1	0	1.261384	2.828392	-1.891035
30	1	0	2.413310	1.666461	-2.585622
31	1	0	0.814271	1.107518	-2.044536

TS: 1,3-dmt $2CH_3OH$ --> 3-mt + $CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -863.118988 (Hartree/particle)
Sum of electronic and thermal Free Energies= -863.161960 (Hartree/particle)
1 imaginary frequency (590.7705i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.493937	-0.178541	-1.076979
2	6	0	2.183333	0.457972	-0.105250
3	6	0	2.309748	-0.355333	1.095292
4	6	0	1.719622	-1.561311	1.000607
5	16	0	0.981678	-1.773305	-0.571038
6	1	0	2.826915	-0.014288	1.984735
7	6	0	-1.078243	-1.076472	0.023617
8	1	0	-1.385624	-2.004462	0.486371
9	1	0	-0.626763	-0.302337	0.627283
10	1	0	-1.358073	-0.884392	-1.002816
11	8	0	-2.834374	-0.225248	0.576800
12	1	0	-2.651835	0.665917	0.207288
13	8	0	-1.662809	1.977873	-0.485279
14	1	0	-1.124548	1.647453	-1.215043
15	6	0	-3.958219	-0.819961	-0.071609
16	1	0	-4.063744	-1.830656	0.320018
17	1	0	-4.860699	-0.248852	0.152936
18	1	0	-3.807407	-0.859124	-1.153518
19	6	0	-0.819528	2.605443	0.481274
20	1	0	-0.240624	3.410274	0.023165
21	1	0	-1.472509	3.026154	1.244914
22	1	0	-0.141361	1.885269	0.948730
23	1	0	1.238638	0.167266	-2.069643
24	6	0	2.747446	1.839063	-0.212006
25	1	0	2.430189	2.448410	0.637983
26	1	0	3.840432	1.806871	-0.197050
27	1	0	2.428391	2.327081	-1.133332
28	1	0	1.650657	-2.353852	1.732738

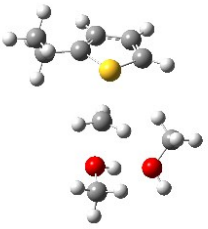


TS: 2e1-mt $2CH_3OH$ --> 2-et + $CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -902.394782 (Hartree/particle)
Sum of electronic and thermal Free Energies= -902.441088 (Hartree/particle)
1 imaginary frequency (587.5564i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.750447	-1.872714	0.807556
2	6	0	1.312700	-2.334296	-0.327374
3	6	0	2.085840	-1.335870	-1.032567
4	6	0	2.111133	-0.127648	-0.428369
5	16	0	1.176003	-0.198243	1.069505
6	1	0	1.194636	-3.352951	-0.675593



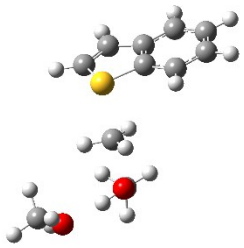
7	1	0	2.594359	-1.527005	-1.970196
8	6	0	-0.680616	0.748676	0.217684
9	1	0	-0.241486	1.736164	0.175616
10	1	0	-0.635698	0.105007	-0.649971
11	1	0	-1.275483	0.472259	1.076784
12	6	0	2.755141	1.153452	-0.852535
13	1	0	3.225186	0.972017	-1.822118
14	1	0	1.981127	1.912411	-1.013703
15	8	0	-2.346120	1.543100	-0.608645
16	1	0	-2.907488	0.743156	-0.738138
17	8	0	-3.759598	-0.734101	-0.618141
18	1	0	-4.620279	-0.606084	-0.201387
19	6	0	-3.004891	2.413332	0.311017
20	1	0	-2.324158	3.233865	0.534776
21	1	0	-3.914151	2.811107	-0.143674
22	1	0	-3.258875	1.884424	1.233726
23	6	0	-3.040742	-1.761622	0.067927
24	1	0	-3.609596	-2.693604	0.064342
25	1	0	-2.106096	-1.913143	-0.470699
26	1	0	-2.825811	-1.470936	1.099562
27	1	0	0.137938	-2.388340	1.533702
28	6	0	3.787576	1.674448	0.148225
29	1	0	4.257232	2.582655	-0.234410
30	1	0	3.329319	1.920034	1.109818
31	1	0	4.569489	0.932323	0.324372

TS: 1-mbt $2CH_3OH$ --> bt + $CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -977.419724 (Hartree/particle)
Sum of electronic and thermal Free Energies= -977.465736 (Hartree/particle)
1 imaginary frequency (594.0200i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.935992	0.194689	-0.592377
2	6	0	-2.390533	0.568698	0.681436
3	6	0	-1.627897	1.675437	1.235962
4	6	0	-0.649858	2.108249	0.425745
5	16	0	-0.580178	1.207940	-1.087593
6	1	0	-1.829097	2.107597	2.208972
7	6	0	1.092652	-0.212526	-0.522460
8	1	0	1.815330	0.587721	-0.434717
9	1	0	0.537807	-0.536208	0.347716
10	6	0	-2.500512	-0.849919	-1.313988
11	1	0	-2.134013	-1.122180	-2.297367
12	6	0	-3.560897	-1.532901	-0.729263
13	1	0	-4.026379	-2.351918	-1.265802
14	6	0	-3.461027	-0.128812	1.247022
15	1	0	-3.831174	0.147997	2.228164
16	6	0	-4.036349	-1.173428	0.537106
17	1	0	-4.867385	-1.719919	0.968759
18	1	0	3.353349	-1.107929	-0.337669
19	8	0	2.525780	-1.513325	0.013660
20	1	0	1.011791	-0.756360	-1.452028
21	6	0	2.630672	-1.596024	1.435893
22	1	0	1.741851	-2.108429	1.802088
23	1	0	3.515467	-2.174412	1.707910
24	1	0	2.689111	-0.598946	1.881423
25	1	0	0.061447	2.906747	0.585251

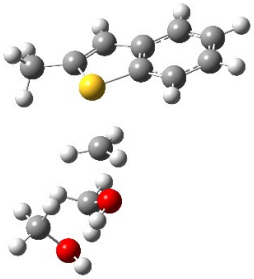


26	8	0	4.764264	-0.221358	-0.689913
27	1	0	4.703149	0.257400	-1.524840
28	6	0	5.171006	0.672347	0.348350
29	1	0	4.431724	1.462430	0.501129
30	1	0	5.263066	0.082763	1.259401
31	1	0	6.138864	1.119213	0.112561

TS: 1,2-dmbt 2CH_3OH --> 2-mbt + $CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -1016.702952 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1016.751341 (Hartree/particle)
1 imaginary frequency (599.0402i cm-1)

Standard orientation:

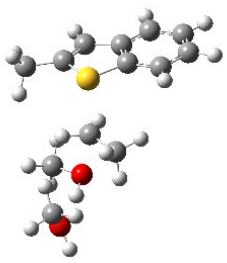


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.791313	-0.323608	-0.630371
2	6	0	-2.508650	0.359014	0.364017
3	6	0	-1.968237	1.681574	0.625865
4	6	0	-0.895434	2.002286	-0.118084
5	16	0	-0.464341	0.673726	-1.221835
6	1	0	-2.389320	2.357186	1.361893
7	6	0	1.162747	-0.228475	0.067746
8	1	0	1.863869	0.557726	-0.175861
9	1	0	0.531608	-0.144039	0.942032
10	6	0	-2.112400	-1.611348	-1.039527
11	1	0	-1.545054	-2.118339	-1.811988
12	6	0	-3.196265	-2.229132	-0.424426
13	1	0	-3.474107	-3.234259	-0.720374
14	6	0	-3.597368	-0.279365	0.964011
15	1	0	-4.169009	0.229864	1.732244
16	6	0	-3.930836	-1.567148	0.565520
17	1	0	-4.773490	-2.068766	1.027888
18	1	0	3.319813	-1.208323	0.690834
19	8	0	2.537572	-1.039081	1.268535
20	1	0	1.169548	-1.146690	-0.502074
21	6	0	2.917677	-0.115037	2.287978
22	1	0	2.059460	0.024704	2.944036
23	1	0	3.749530	-0.524673	2.863190
24	1	0	3.208706	0.845838	1.854651
25	8	0	4.687737	-1.174126	-0.298391
26	1	0	4.900873	-2.024011	-0.701670
27	6	0	4.528313	-0.184585	-1.316590
28	1	0	3.698822	-0.434222	-1.982373
29	1	0	4.320346	0.759299	-0.813989
30	1	0	5.445856	-0.082191	-1.898935
31	6	0	-0.064363	3.238523	-0.122996
32	1	0	0.978083	3.017546	0.123849
33	1	0	-0.079883	3.724285	-1.101630
34	1	0	-0.451901	3.938910	0.617627

TS: 1e2-mbt 2CH_3OH --> 2-mbt + CH_3 $CH_2OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -1055.982560 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1056.032558 (Hartree/particle)
1 imaginary frequency (547.3320i cm-1)

Standard orientation:



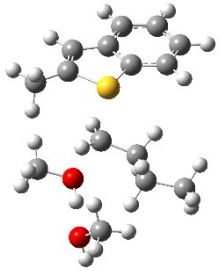
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.971416	-0.389349	-0.543838
2	6	0	-2.552688	0.511031	0.364307
3	6	0	-1.925656	1.819298	0.320316
4	6	0	-0.921997	1.923312	-0.569629
5	16	0	-0.662486	0.387095	-1.425468
6	1	0	-2.233838	2.645553	0.950984
7	6	0	1.099853	-0.246960	0.025734
8	1	0	1.697007	0.538937	-0.416744
9	1	0	0.429695	0.009172	0.835469
10	6	0	-2.409173	-1.701681	-0.681962
11	1	0	-1.955128	-2.376099	-1.399167
12	6	0	-3.458918	-2.119676	0.128397
13	1	0	-3.822163	-3.137643	0.045642
14	6	0	-3.610703	0.069644	1.164428
15	1	0	-4.076833	0.748770	1.870066
16	6	0	-4.052530	-1.240792	1.041832
17	1	0	-4.872175	-1.589130	1.660216
18	1	0	3.348509	-0.544651	1.194254
19	8	0	2.502214	-0.197252	1.560517
20	6	0	2.694838	1.162941	1.941879
21	1	0	1.714008	1.591720	2.151376
22	1	0	3.306552	1.215327	2.844669
23	1	0	3.177695	1.729853	1.141510
24	8	0	4.752595	-0.883743	0.322679
25	1	0	5.356135	-1.588363	0.585189
26	6	0	4.573673	-0.892735	-1.093447
27	1	0	4.272143	-1.880511	-1.447140
28	1	0	3.789586	-0.170870	-1.321768
29	1	0	5.493903	-0.589880	-1.597733
30	6	0	-0.023397	3.074576	-0.866583
31	1	0	1.013388	2.845510	-0.600317
32	1	0	-0.044697	3.336553	-1.926999
33	1	0	-0.341556	3.942544	-0.287849
34	6	0	1.274973	-1.664815	-0.405323
35	1	0	1.562358	-1.730569	-1.454390
36	1	0	2.073942	-2.121590	0.184756
37	1	0	0.371626	-2.248961	-0.226780

TS: 1b2-mbt $2CH_3OH$ --> 2-mbt + $CH_3CH_2CH_2CH_2OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -1018.869183 (Hartree/particle)
Sum of electronic and thermal Free Energies= -1134.579283 (Hartree/particle)
1 imaginary frequency (495.9264i cm-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.421991	0.369334	0.755480
2	6	0	1.932470	0.817960	-0.474921
3	6	0	1.086940	1.825416	-1.087574
4	6	0	-0.016348	2.127536	-0.378685
5	16	0	-0.081902	1.194107	1.134521
6	1	0	1.317742	2.296715	-2.036245
7	6	0	-1.893587	-0.366777	0.617462
8	1	0	-2.292541	-0.195889	1.609058
9	1	0	-2.159729	0.335532	-0.161140
10	6	0	2.066120	-0.591393	1.526864



11	1	0	1.662646	-0.913864	2.480412
12	6	0	3.254137	-1.124122	1.036830
13	1	0	3.778050	-1.876771	1.614939
14	6	0	3.125878	0.266459	-0.948030
15	1	0	3.537560	0.597135	-1.895489
16	6	0	3.775494	-0.700136	-0.190033
17	1	0	4.702094	-1.130811	-0.552759
18	6	0	-1.102694	3.104423	-0.674536
19	1	0	-1.143526	3.889624	0.084433
20	1	0	-0.918045	3.569650	-1.643534
21	1	0	-2.084211	2.623090	-0.706274
22	6	0	-1.113823	-1.592776	0.305630
23	1	0	-0.293281	-1.697237	1.022731
24	1	0	-1.765042	-2.447804	0.520070
25	1	0	-4.068808	-1.714940	0.868732
26	8	0	-3.792979	-1.174152	0.115928
27	6	0	-4.740238	-0.123724	-0.095437
28	1	0	-4.451533	0.384167	-1.014337
29	1	0	-5.741316	-0.540561	-0.212853
30	1	0	-4.729585	0.584442	0.736544
31	6	0	-0.606360	-1.632941	-1.133075
32	1	0	-0.182559	-0.659730	-1.398682
33	1	0	-1.456814	-1.792515	-1.803554
34	6	0	0.442987	-2.717789	-1.333688
35	1	0	0.047616	-3.704096	-1.073873
36	1	0	0.779531	-2.755720	-2.372119
37	1	0	1.318206	-2.531753	-0.703552

Methanolysis byproducts

2,5-dmt (in methanol)

Sum of electronic and zero-point Energies= -631.459517 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.490933 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.259744	-0.125966	0.000020
2	6	0	0.716060	-1.374699	-0.000087
3	6	0	-0.716061	-1.374698	0.000069
4	6	0	-1.259744	-0.125965	-0.000001
5	16	0	0.000000	1.075708	-0.000017
6	1	0	1.322392	-2.273666	-0.000138
7	1	0	-1.322392	-2.273666	0.000107
8	6	0	-2.703337	0.265167	-0.000001
9	1	0	-2.963680	0.856597	0.881707
10	1	0	-2.963705	0.856555	-0.881732
11	1	0	-3.324881	-0.632162	0.000031
12	6	0	2.703337	0.265166	0.000032
13	1	0	2.963689	0.856592	-0.881677
14	1	0	2.963696	0.856560	0.881762
15	1	0	3.324881	-0.632162	0.000012

3-mt (in metanol)

Sum of electronic and zero-point Energies= -592.180800 (Hartree/particle)

Sum of electronic and thermal Free Energies= -592.211170 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035859	1.147027	-0.000173
2	6	0	-0.321363	1.244860	0.000149
3	6	0	-0.979783	-0.030217	-0.000073
4	6	0	-0.080638	-1.056151	-0.000053
5	16	0	1.553616	-0.497477	0.000060
6	1	0	-0.850927	2.190530	0.000269
7	1	0	-0.285431	-2.118020	-0.000053
8	1	0	1.766255	1.943874	-0.000259
9	6	0	-2.470958	-0.197061	-0.000009
10	1	0	-2.918363	0.271955	0.880282
11	1	0	-2.918494	0.272381	-0.880004
12	1	0	-2.749603	-1.251831	-0.000234

2-et (in methanol)

Sum of electronic and zero-point Energies= -631.455159 (Hartree/particle)
Sum of electronic and thermal Free Energies= -631.487113 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.016891	-0.440216	0.171360
2	6	0	1.924809	0.916007	0.227815
3	6	0	0.592822	1.384687	-0.002255
4	6	0	-0.305778	0.383065	-0.230764
5	16	0	0.484840	-1.163857	-0.160765
6	1	0	2.770173	1.562688	0.428798
7	1	0	0.309852	2.431285	-0.000050
8	6	0	-1.778318	0.495352	-0.495822
9	1	0	-2.010755	0.089833	-1.485763
10	1	0	-2.024657	1.560054	-0.527086
11	6	0	-2.636674	-0.206476	0.558031
12	1	0	-3.698181	-0.047090	0.355265
13	1	0	-2.458449	-1.284922	0.565315
14	1	0	-2.417906	0.178243	1.557222
15	1	0	2.889976	-1.062897	0.308353

Bt (in metanol)

Sum of electronic and zero-point Energies= -706.479639 (Hartree/particle)
Sum of electronic and thermal Free Energies= -706.510632 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.109426	0.847375	0.000063
2	6	0	-0.062143	-0.551281	-0.000037
3	6	0	1.028414	-1.425475	0.000061
4	6	0	2.302171	-0.882225	0.000255

5	6	0	2.493040	0.510354	0.000355
6	6	0	1.411912	1.372676	0.000260
7	6	0	-1.152763	1.545399	-0.000067
8	6	0	-2.211104	0.705094	-0.000253
9	1	0	0.880986	-2.499791	-0.000016
10	1	0	3.163103	-1.541422	0.000332
11	1	0	3.500960	0.909877	0.000510
12	1	0	1.560387	2.447496	0.000335
13	1	0	-1.242039	2.624635	-0.000021
14	1	0	-3.261330	0.963140	-0.000374
15	16	0	-1.757236	-0.977215	-0.000286

2-mbt (in methanol)

Sum of electronic and zero-point Energies= -745.760465 (Hartree/particle)
Sum of electronic and thermal Free Energies= -745.794022 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.399643	0.792654	-0.000088
2	6	0	-0.427604	-0.616026	-0.000047
3	6	0	-1.628897	-1.327447	-0.000169
4	6	0	-2.815900	-0.610666	-0.000325
5	6	0	-2.808257	0.793537	-0.000362
6	6	0	-1.614544	1.495053	-0.000247
7	6	0	0.948447	1.305491	0.000060
8	6	0	1.896089	0.338761	0.000213
9	1	0	-1.636166	-2.412134	-0.000140
10	1	0	-3.760363	-1.143683	-0.000420
11	1	0	-3.749157	1.332947	-0.000484
12	1	0	-1.610215	2.580335	-0.000276
13	1	0	1.186834	2.363295	0.000058
14	16	0	1.192373	-1.271129	0.000177
15	6	0	3.381624	0.495105	0.000445
16	1	0	3.831011	0.032062	0.882599
17	1	0	3.831376	0.031566	-0.881259
18	1	0	3.640824	1.554904	0.000213

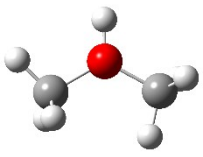
CH_3OHCH_3 (in methanol)

Sum of electronic and zero-point Energies= -155.308848 (Hartree/particle)
Sum of electronic and thermal Free Energies= -155.334811 (Hartree/particle)

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.274559	-0.234652	0.000000
2	1	0	-1.031626	-1.293253	0.000000
3	1	0	-1.807880	0.049392	0.902577
4	1	0	-1.807880	0.049391	-0.902576
5	8	0	0.000123	0.468774	0.000000
6	1	0	-0.001661	1.438506	0.000000
7	6	0	1.272297	-0.238583	0.000000



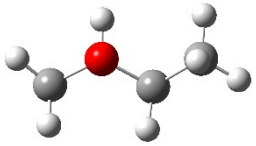
8	1	0	2.041614	0.527621	-0.000001
9	1	0	1.310011	-0.841218	0.903582
10	1	0	1.310010	-0.841220	-0.903580

$CH_3CH_2OHCH_3$ (in methanol)

Sum of electronic and zero-point Energies= -194.593575 (Hartree/particle)
Sum of electronic and thermal Free Energies= -194.621722 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.514889	-0.452936	-0.040391
2	6	0	0.575662	0.546888	0.094039
3	1	0	0.445973	1.016687	1.068351
4	1	0	0.369727	1.256904	-0.703699
5	6	0	1.890101	-0.160164	-0.069237
6	1	0	2.684931	0.584322	0.010901
7	1	0	2.043454	-0.904609	0.714587
8	1	0	1.961770	-0.638495	-1.046722
9	6	0	-1.875032	0.092007	-0.048933
10	1	0	-1.945353	0.699078	-0.946184
11	1	0	-2.540838	-0.764245	-0.094627
12	1	0	-2.022094	0.676396	0.856869
13	1	0	-0.422836	-1.174936	0.608429

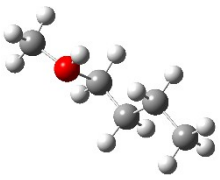


$CH_3CH_2CH_2CH_2OHCH_3$ (in methanol)

Sum of electronic and zero-point Energies= -273.140370 (Hartree/particle)
Sum of electronic and thermal Free Energies= -273.172484 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.463259	-0.392853	-0.215514
2	6	0	-0.704428	0.787866	0.279383
3	1	0	-0.776364	0.763392	1.367342
4	1	0	-1.261429	1.631996	-0.121648
5	6	0	0.708044	0.733179	-0.240494
6	1	0	1.155566	1.694662	0.035674
7	1	0	0.686785	0.698632	-1.334249
8	6	0	-2.917498	-0.316083	-0.046835
9	1	0	-3.247424	0.500609	-0.681193
10	1	0	-3.309986	-1.268682	-0.388931
11	1	0	-3.137301	-0.135843	1.003461
12	1	0	-1.116780	-1.228723	0.145459
13	6	0	1.558422	-0.402834	0.324075
14	1	0	1.154021	-1.372400	0.012532
15	1	0	1.514574	-0.376958	1.418045
16	6	0	3.006317	-0.296167	-0.140746
17	1	0	3.453419	0.646211	0.187940
18	1	0	3.613115	-1.111618	0.259135
19	1	0	3.072726	-0.334215	-1.231751

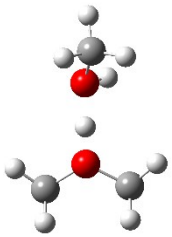


$CH_3OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -270.987220 (Hartree/particle)
Sum of electronic and thermal Free Energies= -271.019785 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.443991	1.259188	0.030399
2	1	0	-2.358810	1.357497	-0.549987
3	1	0	-0.729415	2.031639	-0.243537
4	1	0	-1.652106	1.277775	1.100570
5	8	0	-0.837914	-0.005038	-0.318885
6	1	0	0.187469	-0.092249	0.096768
7	8	0	1.397567	-0.194911	0.587329
8	1	0	1.507263	0.402108	1.340053
9	6	0	-1.652134	-1.157952	-0.003153
10	1	0	-2.565725	-1.085488	-0.589336
11	1	0	-1.076016	-2.033078	-0.292616
12	1	0	-1.869501	-1.164387	1.065101
13	6	0	2.434837	0.020255	-0.390592
14	1	0	3.403707	-0.141921	0.078222
15	1	0	2.275797	-0.711854	-1.178673
16	1	0	2.367846	1.030605	-0.794038

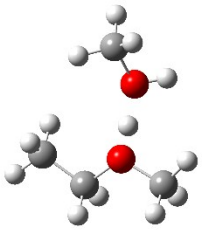


$CH_2OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -310.267201 (Hartree/particle)
Sum of electronic and thermal Free Energies= -310.302380 (Hartree/particle)
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.287819	1.779728	-0.129967
2	1	0	-2.201753	1.803678	-0.718830
3	1	0	-0.562043	2.490366	-0.517861
4	1	0	-1.493315	1.962875	0.924804
5	8	0	-0.701199	0.465893	-0.284998
6	1	0	0.306090	0.431883	0.132858
7	8	0	1.561242	0.337170	0.604047
8	1	0	1.870880	1.168411	0.987573
9	6	0	-1.534516	-0.632822	0.202257
10	1	0	-2.466296	-0.561192	-0.357868
11	1	0	-1.724355	-0.452797	1.262212
12	6	0	2.495325	-0.152673	-0.375450
13	1	0	3.452060	-0.346919	0.106887
14	1	0	2.081818	-1.080319	-0.765542
15	1	0	2.614523	0.571878	-1.181302
16	6	0	-0.811323	-1.930289	-0.048366
17	1	0	0.123242	-1.979608	0.514006
18	1	0	-1.447811	-2.753640	0.281381
19	1	0	-0.603384	-2.062786	-1.111558



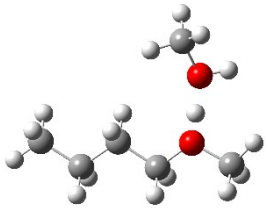
$CH_3CH_2CH_2CH_2OH(OHCH_3)CH_3$ (in methanol)

Sum of electronic and zero-point Energies= -388.814725 (Hartree/particle)
Sum of electronic and thermal Free Energies= -388.852978 (Hartree/particle)

No imaginary frequencies

Standard orientation:

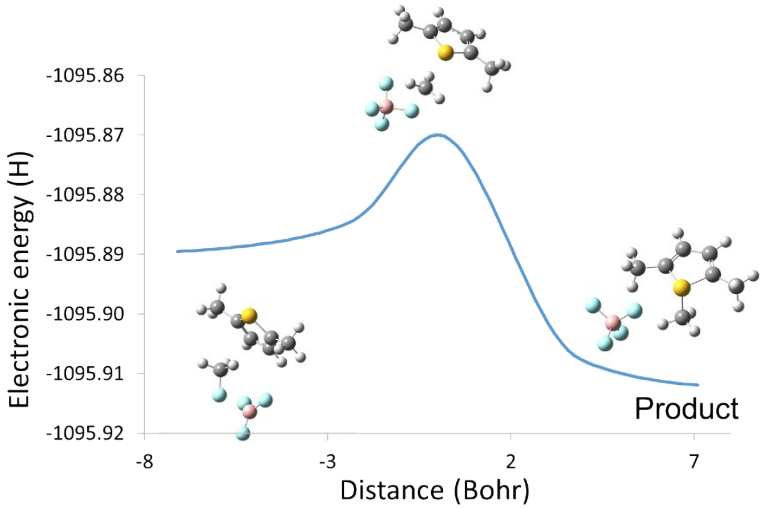
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.092732	-1.955745	-0.100320
2	1	0	-1.776944	-2.824337	-0.673276
3	1	0	-3.044669	-1.578888	-0.466080
4	1	0	-2.139848	-2.180339	0.965261
5	8	0	-1.120154	-0.906729	-0.326056
6	1	0	-1.471548	0.026061	0.093810
7	8	0	-1.903065	1.208893	0.608549
8	1	0	-2.790859	1.141734	0.984507
9	6	0	0.231289	-1.229640	0.128829
10	1	0	0.510592	-2.134533	-0.411709
11	1	0	0.173175	-1.440434	1.199532
12	6	0	-1.827491	2.302317	-0.323113
13	1	0	-2.002443	3.238363	0.205467
14	1	0	-0.820240	2.293046	-0.734295
15	1	0	-2.557968	2.172731	-1.121903
16	6	0	1.144702	-0.068631	-0.185764
17	1	0	0.795860	0.826025	0.341428
18	1	0	1.104653	0.140115	-1.259592
19	6	0	2.580173	-0.385838	0.231162
20	1	0	2.917522	-1.287350	-0.290837
21	1	0	2.606184	-0.613701	1.301879
22	6	0	3.526171	0.770108	-0.073286
23	1	0	3.230888	1.673493	0.467913
24	1	0	4.552344	0.529229	0.214239
25	1	0	3.526383	1.006053	-1.141340



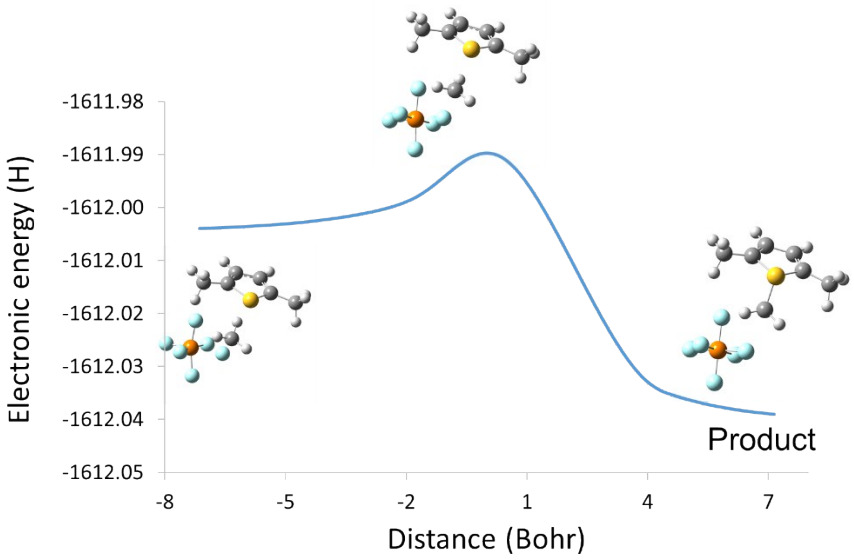
IRCs

Synthesis Reaction coordinates

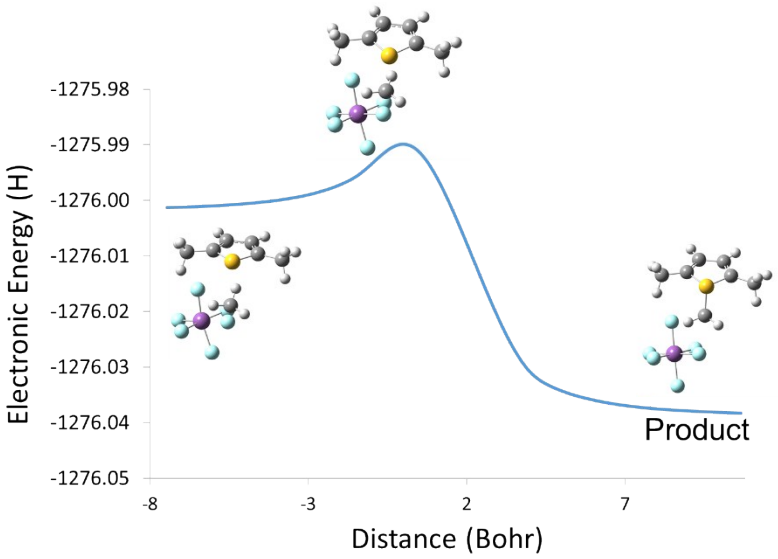
$F_3B\text{-}F\text{-}CH_3$ + 2,5- dmt --> 1,2,5-tmt BF_4



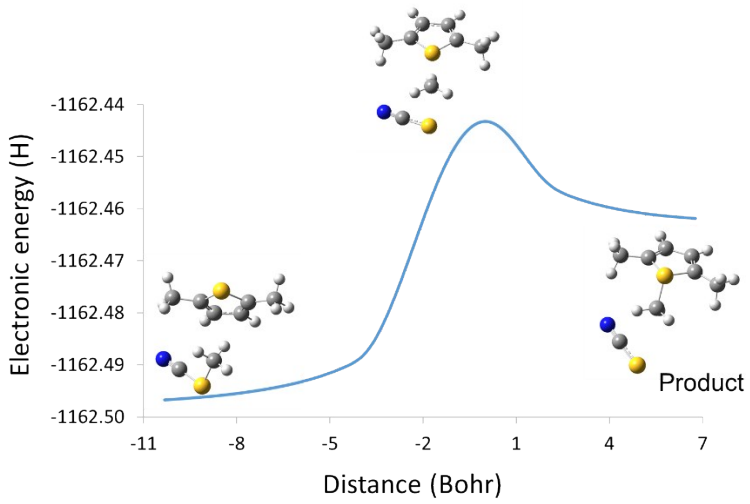
F_5P-F-CH_3 + 2,5- dmt --> 1,2,5-tmt PF_6



$F_5Sb\text{-}F\text{-}CH_3$ + 2,5- dmt --> 1,2,5-tmt SbF_6

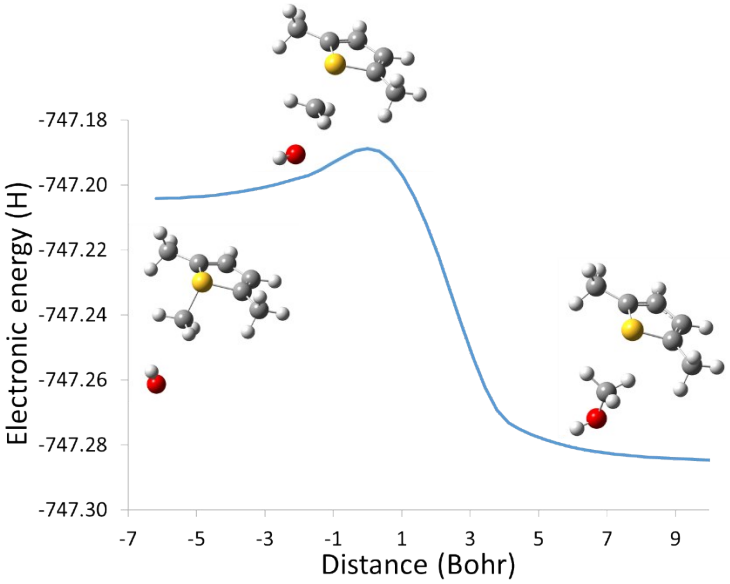


$NCS\text{-}CH_3$ + 2,5- dmt --> 1,2,5-tmt SbF_6

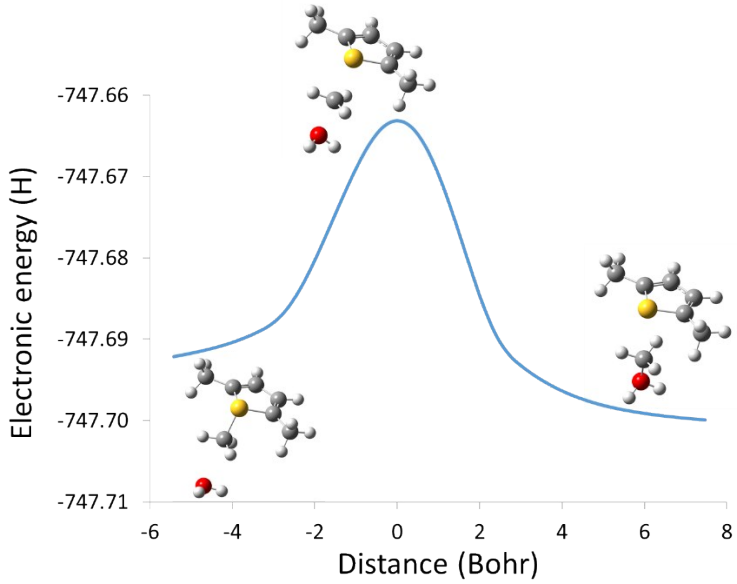


Sovolysis Reaction coordinates

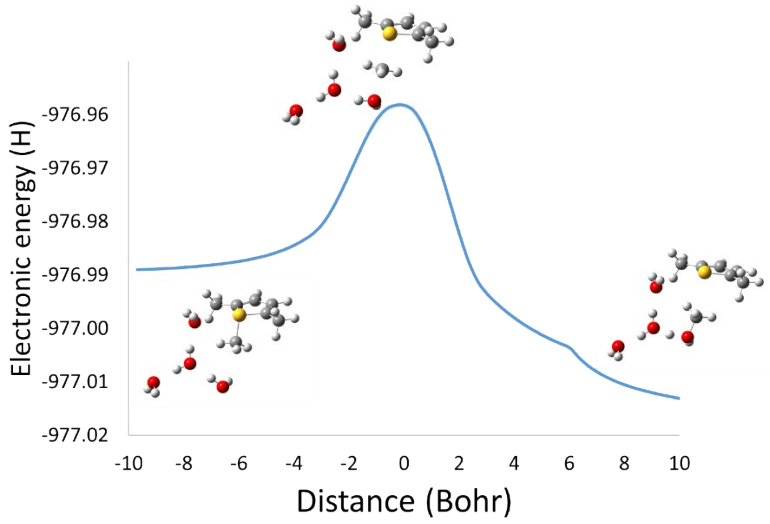
1,2,5-tmt OH --> 2,5-dmt + CH_3OH



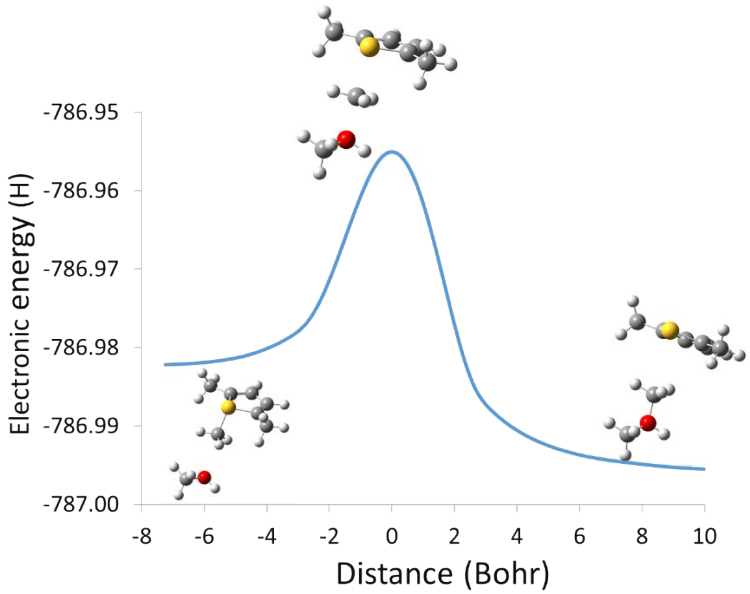
1,2,5-tmt H2O --> 2,5-dmt + CH3OH2



1,2,5-tmt 4 H_2O --> 2,5-dmt + CH_3OH H_3O^+ $2H_2O$



1,2,5-tmt CH3OH --> 2,5-dmt + CH3OHCH3



1,2,5-tmt $2CH_3OH$ --> 2,5-dmt + $CH_3OH(OHCH_3)CH_3$