Supplementary Information for

Theoretical study on reaction mechanism of phosphate-catalyzed N-S acyl transfer of *N*-sulfanylethylanilide (SEAlide)

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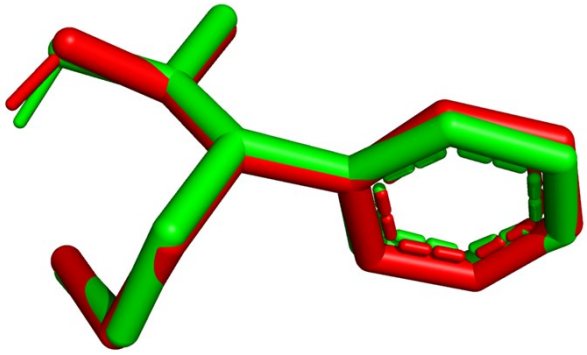


Fig. S1. Overlay of **ts1** optimized in gas phase (green) and water (red). Non-polar hydrogens are omitted for clarity. Images are generated using PyMOL (The PyMOL Molecular Graphics System, Version 4.3. Schrödinger, LCC).

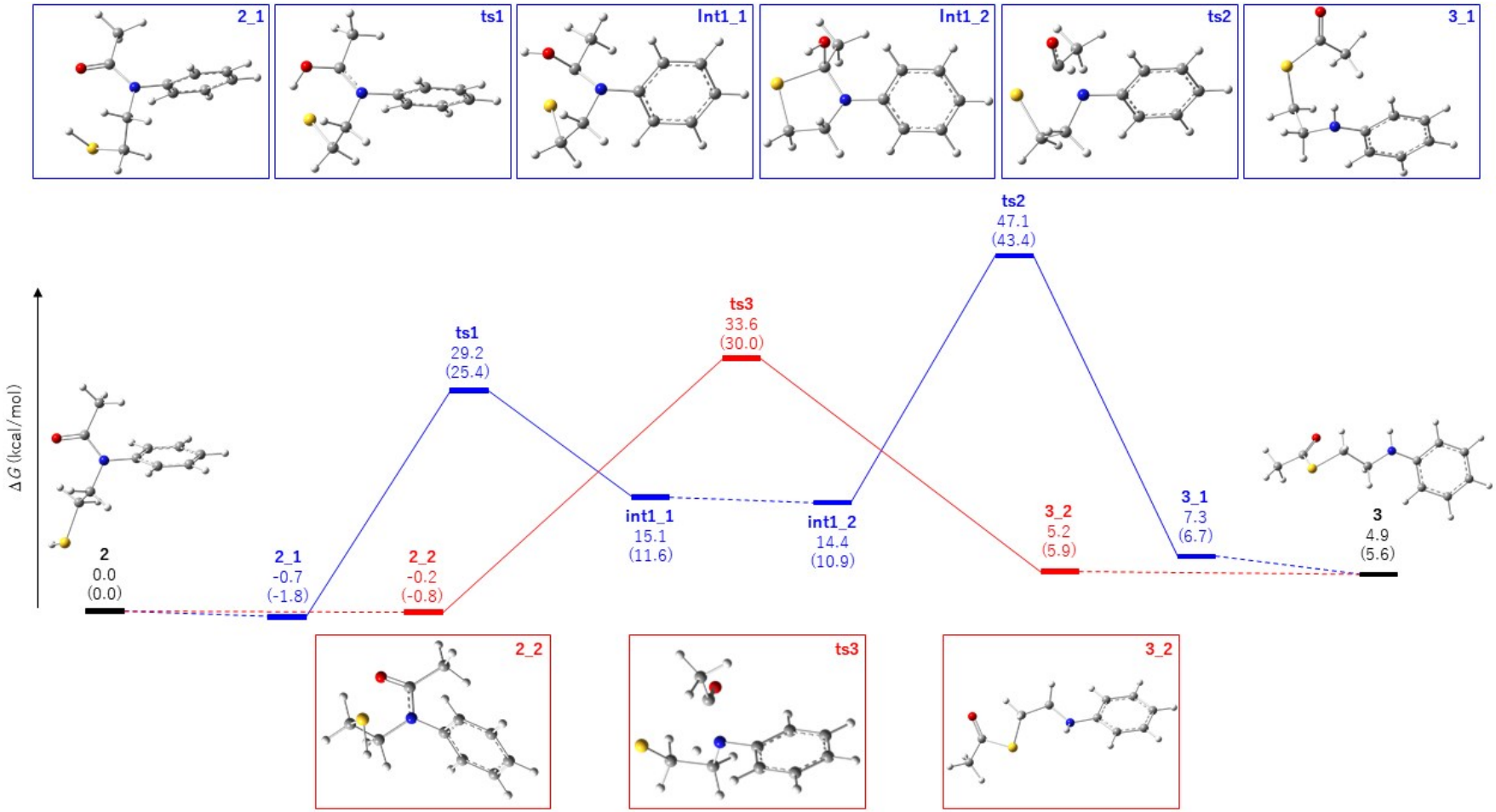


Fig. S2. Calculated Gibbs free energy profile of a reaction depicted in Scheme 2 (blue: stepwise mechanism; red: concerted mechanism) and optimized structures (H: white; C: grey; N: blue; O: red; S: yellow). Compound number **x_n** means the **n** th conformer of **x**. Δ*H* values are shown in parentheses (kcal/mol).

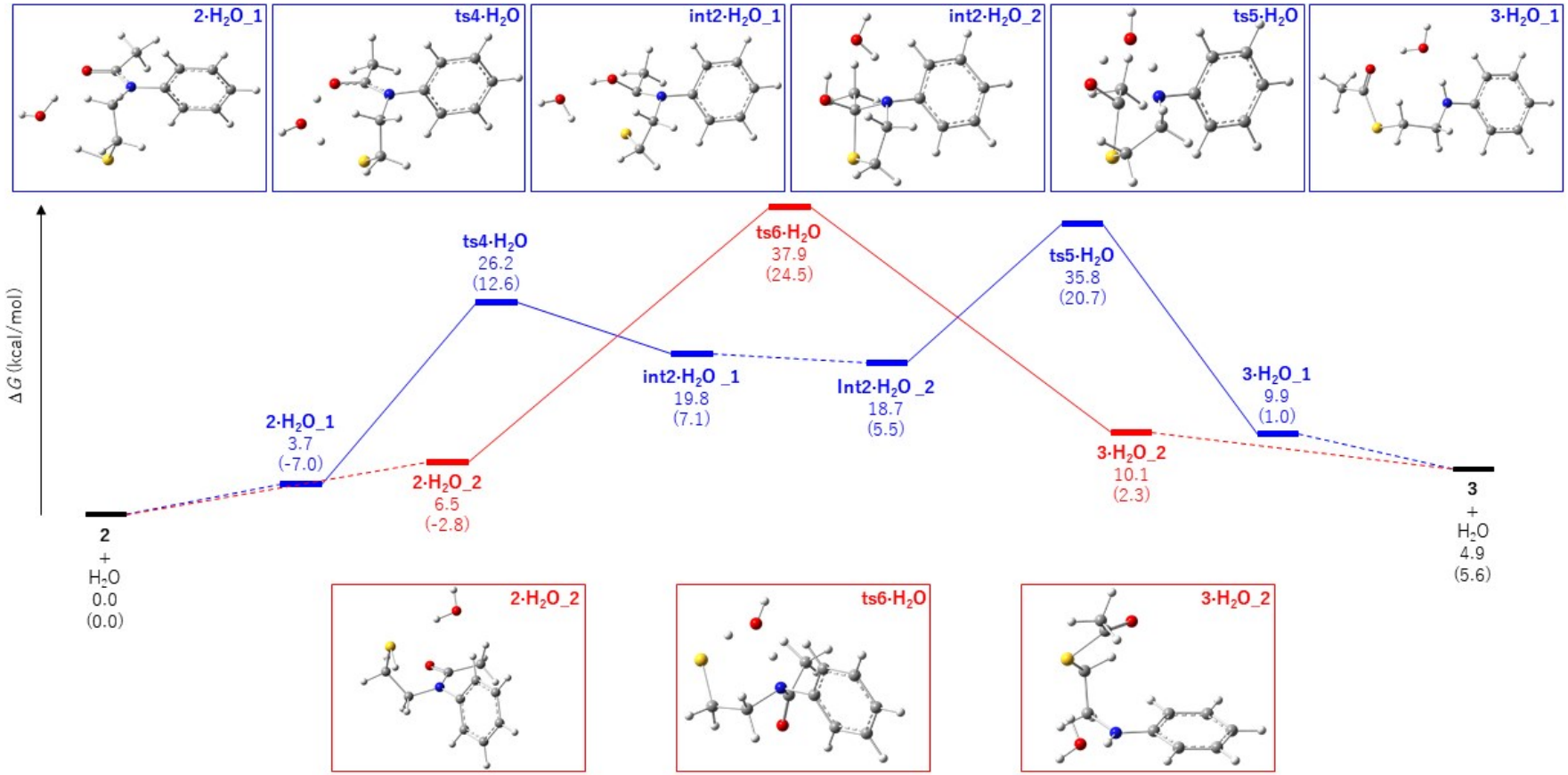


Fig. S3. Calculated Gibbs free energy profile of a reaction in the presence of H_2O depicted in Scheme 3 (blue: stepwise mechanism; red: concerted mechanism) and optimized structures (H: white; C: grey; N: blue; O: red; S: yellow). Compound number **x_n** means the **n** th conformer of **x**. Δ*H* values are shown in parentheses (kcal/mol).

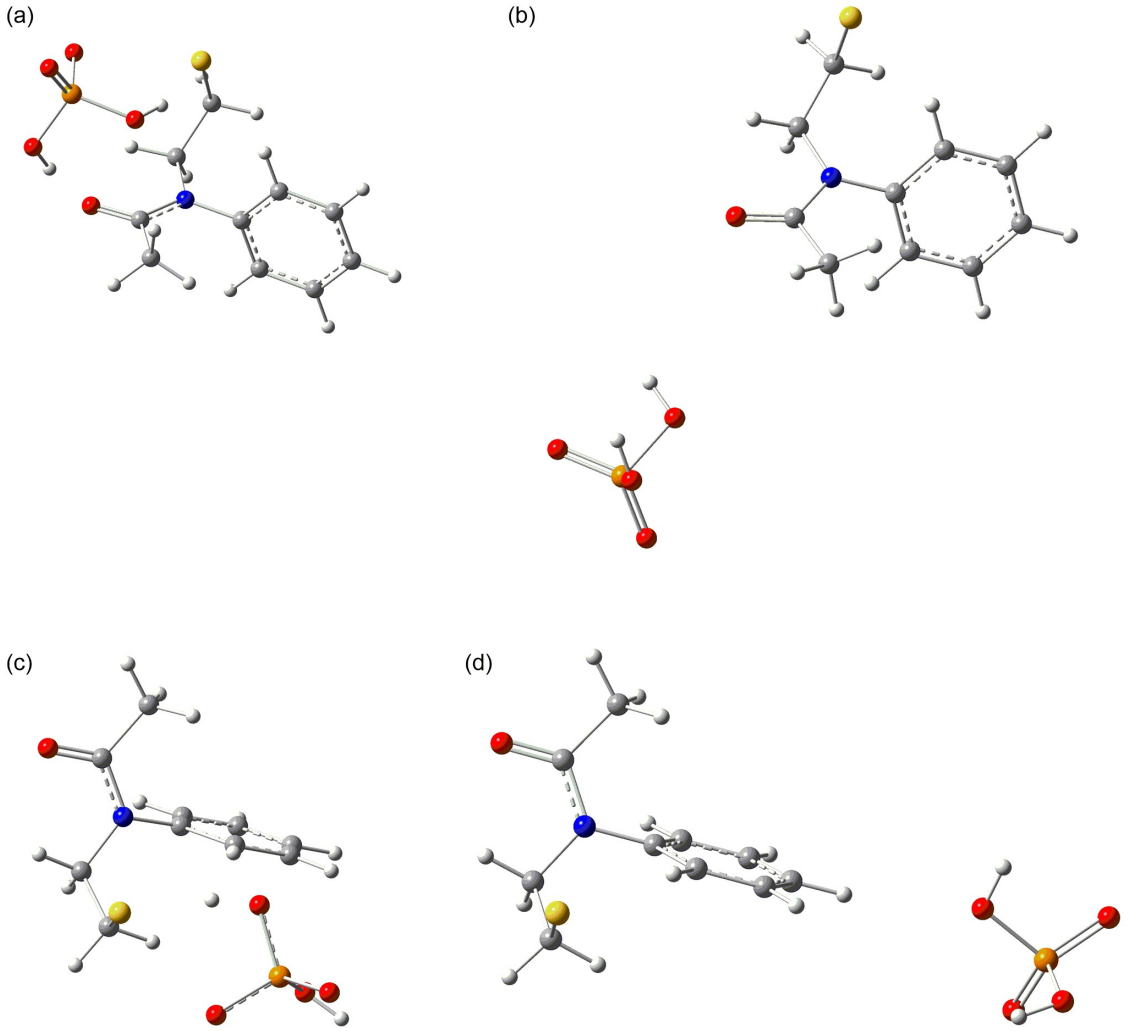


Fig. S4. Structural optimization of **2·HPO_4^{2-}** at B3LYP/6-31+G(d); **2·HPO_4^{2-}_1** (a) before optimization (an optimized structure of **2·$H_2PO_4^-$_1** was diverted) and (b) in the middle of optimization; **2·HPO_4^{2-}_2** (c) before optimization (an optimized structures of **2·$H_2PO_4^-$_2** was diverted) and (d) in the middle of optimization.

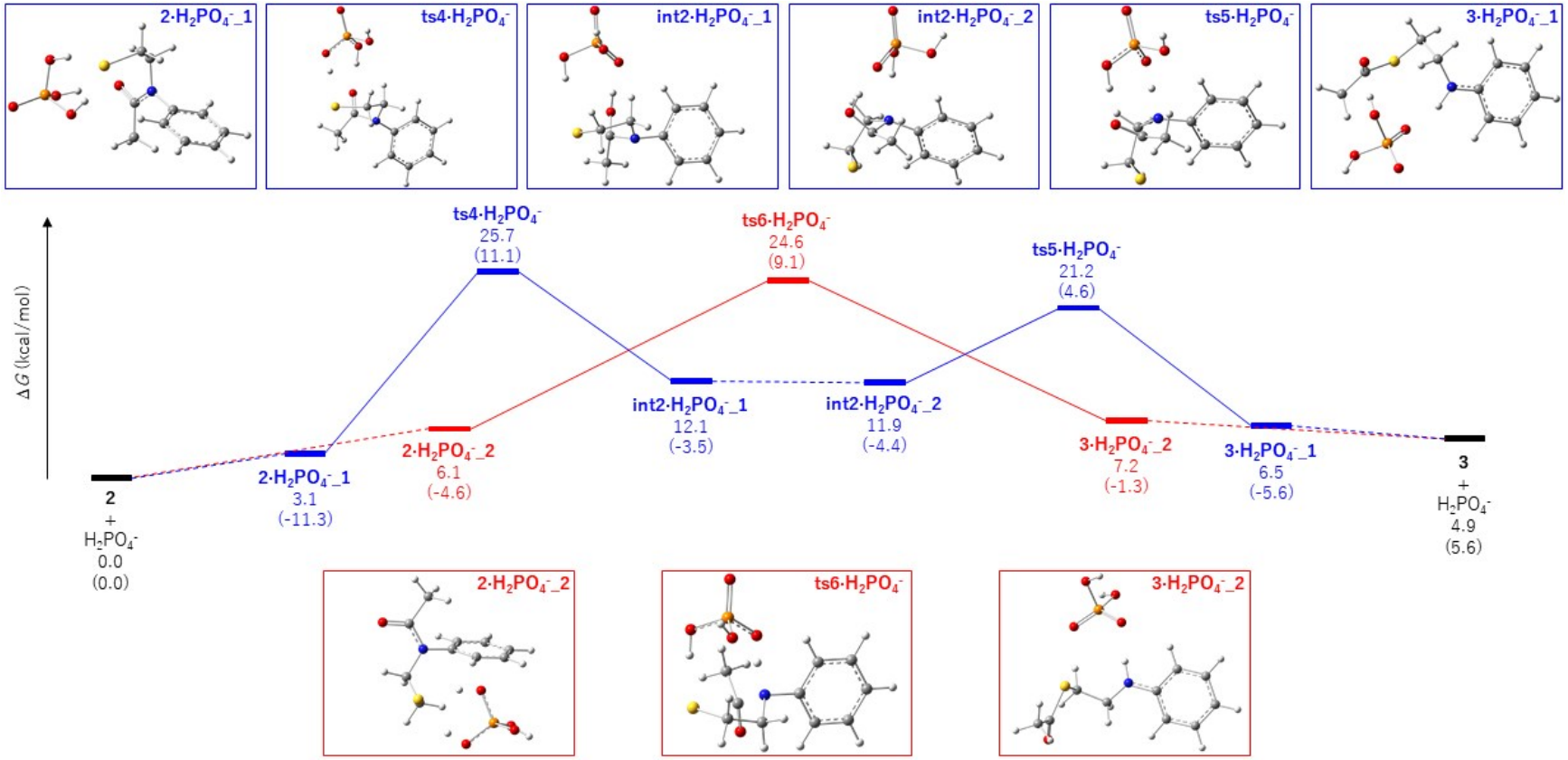


Fig. S5. Calculated Gibbs free energy profile of a reaction in the presence of $H_2PO_4^-$ depicted in Scheme 3 (blue: stepwise mechanism; red: concerted mechanism) and optimized structures (H: white; C: grey; N: blue; O: red; P: orange; S: yellow). Compound number **x_n** means the **n** th conformer of **x**. Δ*H* values are shown in parentheses (kcal/mol).

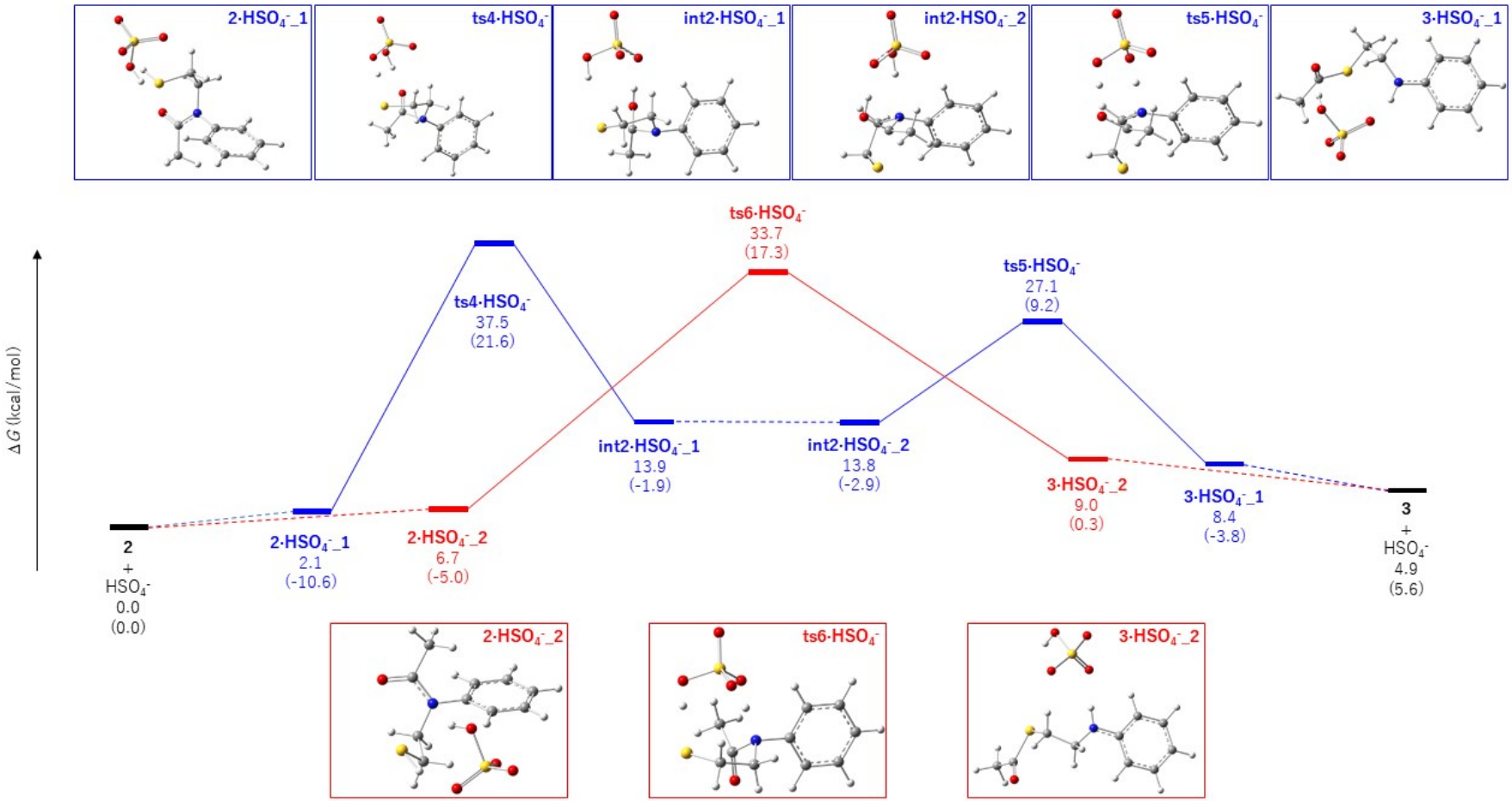


Fig. S6. Calculated Gibbs free energy profile of a reaction in the presence of HSO_4^- depicted in Scheme 3 (blue: stepwise mechanism; red: concerted mechanism) and optimized structures (H: white; C: grey; N: blue; O: red; S: yellow). Compound number **x_n** means the **n** th conformer of **x**. Δ*H* values are shown in parentheses (kcal/mol).

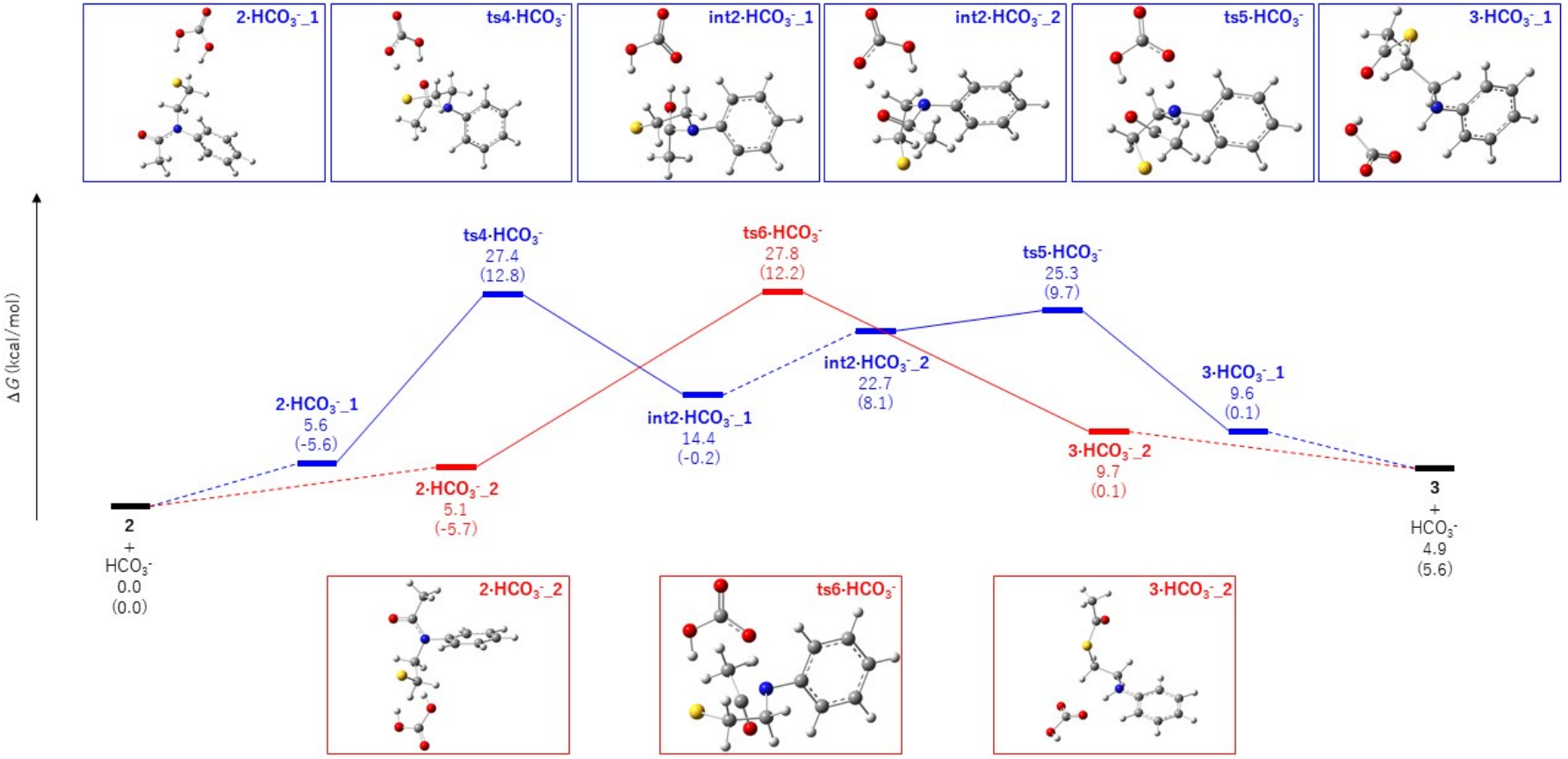


Fig. S7. Calculated Gibbs free energy profile of a reaction in the presence of HCO_3^- depicted in Scheme 3 (blue: stepwise mechanism; red: concerted mechanism) and optimized structures (H: white; C: grey; N: blue; O: red; S: yellow). Compound number **x_n** means the **n** th conformer of **x**. Δ*H* values are shown in parentheses (kcal/mol).

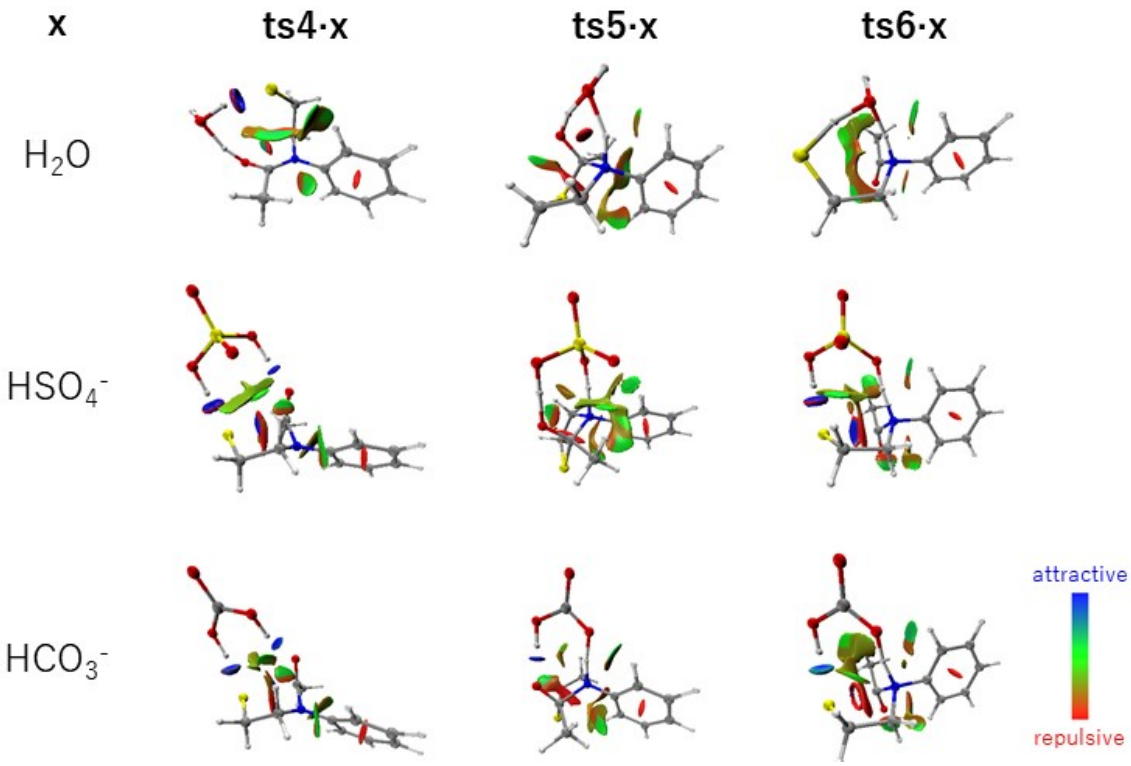


Fig. S8. NCI analyses of **ts4·x**, **ts5·x** and **ts6·x** (H: white; C: grey; N: blue; O: red; S: yellow). Transition states (**x** = $H_2PO_4^-$) are depicted in Fig. S9.

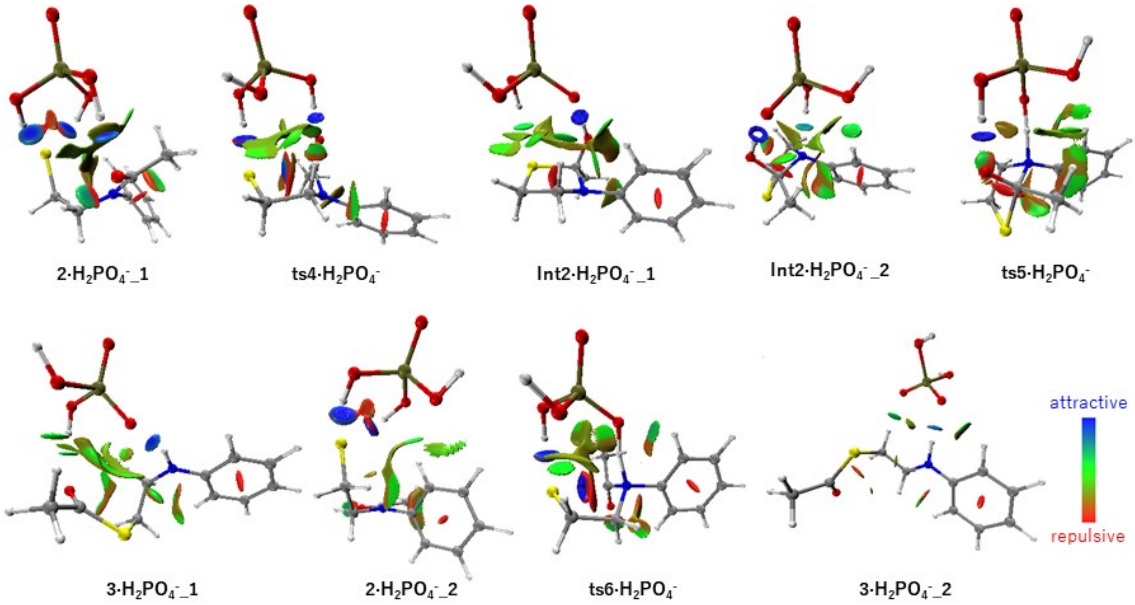


Fig. S9. NCI analyses of intermediates and transition states of the $H_2PO_4^-$-catalysed reaction (H: white; C: grey; N: blue; O: red; P: ochre; S: yellow).

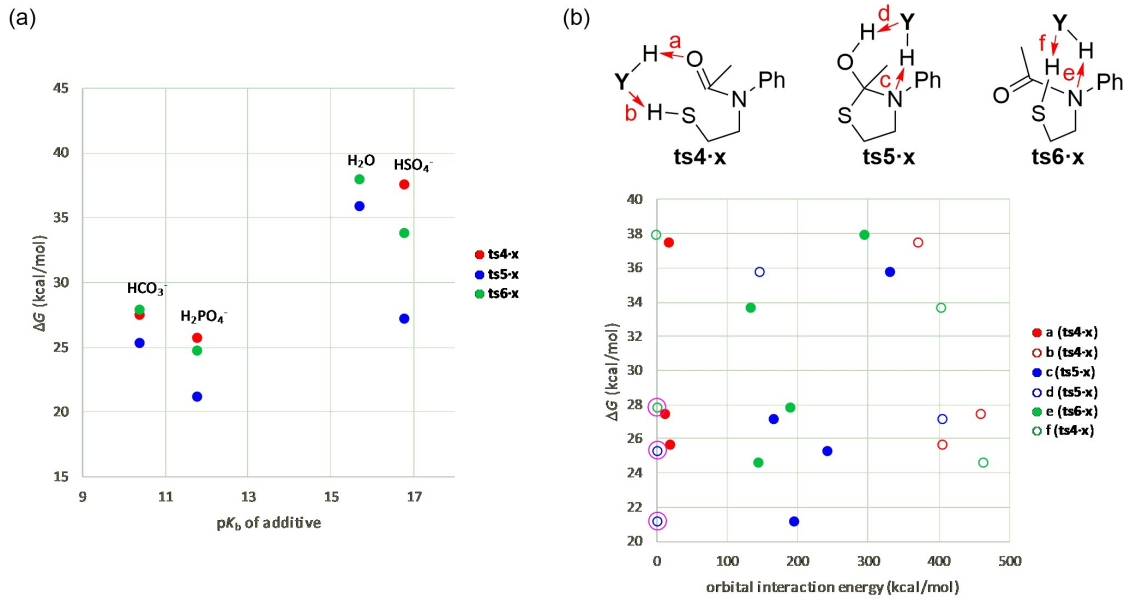
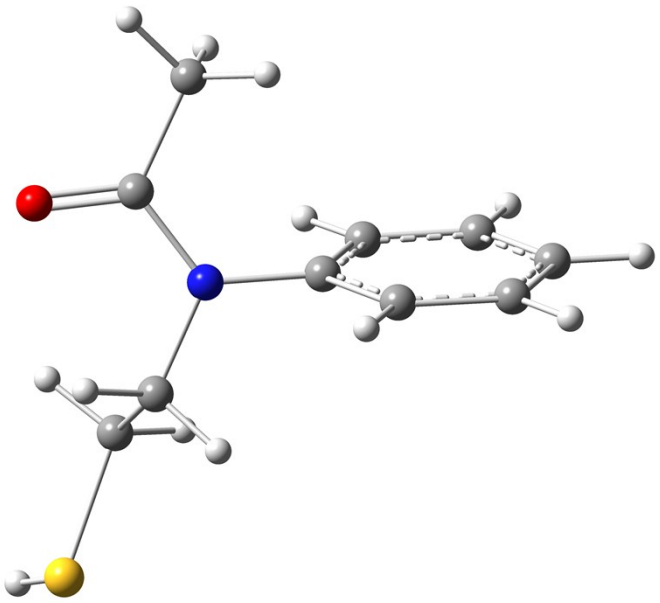


Fig. S10. Relationship between Δ*G* of transition states and (a) pK_b of additives[20,24,27] or (b) sum of donor-acceptor interaction energies estimated using NBO analysis[29] at M06-2X/6-311+G(d,p) (Purple circles: covalent bond). **ts4·H$_2$O** is not plotted because its conformation is quite different to that of other **ts4·x** (Fig. 3).

2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.9897706 hartree/particle

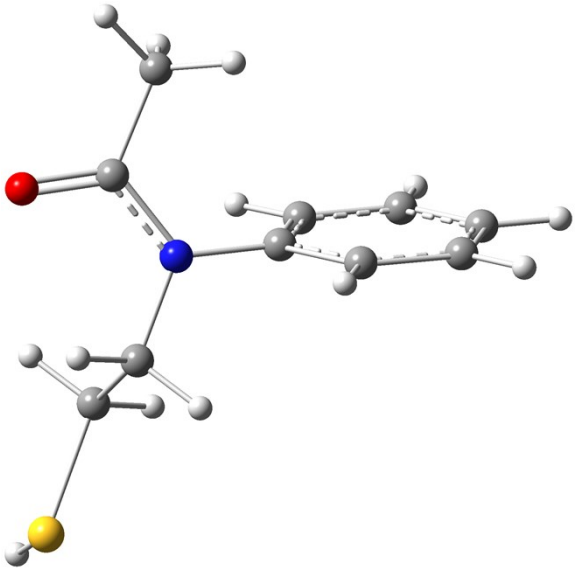
Thermal correction to Gibbs free energy: 0.168964 hartree/particle

Thermal correction to Enthalpy: 0.226025 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.570882	-0.299194	-1.141665
2	6	0	2.750960	-1.033436	-1.289156
3	6	0	3.414347	-1.530263	-0.164245
4	6	0	2.895613	-1.286284	1.111434
5	6	0	1.723227	-0.543211	1.262179
6	6	0	1.056136	-0.043136	0.135352
7	1	0	1.044415	0.077074	-2.014703
8	1	0	3.145109	-1.224084	-2.283981
9	1	0	4.328728	-2.105951	-0.280101
10	1	0	3.407453	-1.668478	1.990785
11	1	0	1.322133	-0.340044	2.251816
12	6	0	-1.380686	-0.040808	0.668153
13	1	0	-1.078729	-0.897704	1.278531
14	1	0	-2.007122	0.620250	1.271290
15	6	0	-2.162907	-0.513566	-0.562455
16	1	0	-1.521907	-1.115921	-1.213178
17	1	0	-2.531663	0.355178	-1.112596
18	16	0	-3.593967	-1.537682	0.006083
19	1	0	-4.211775	-1.614096	-1.191429
20	6	0	-0.267978	2.057787	0.068980
21	6	0	1.008555	2.824210	-0.236869
22	1	0	1.864045	2.478908	0.350615
23	1	0	1.271711	2.723530	-1.296317
24	1	0	0.815424	3.879022	-0.032283
25	8	0	-1.357015	2.624985	0.122864
26	7	0	-0.162446	0.697536	0.298724

2 optimized in PCM (water)



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d) in PCM (water), 1 atm, 298.15 K

Energy: -916.98982617 hartree/particle

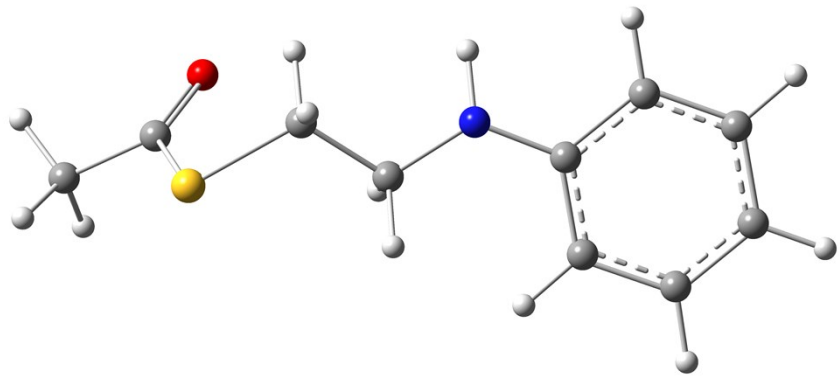
Thermal correction to Gibbs free energy: 0.168834 hartree/particle

Thermal correction to Enthalpy: 0.22592 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.531627	-0.358633	1.141929
2	6	0	-2.703171	-1.110495	1.275369
3	6	0	-3.386214	-1.555239	0.139324
4	6	0	-2.896444	-1.243813	-1.134114
5	6	0	-1.731110	-0.485659	-1.271845
6	6	0	-1.049169	-0.038568	-0.132580
7	1	0	-0.993304	-0.019445	2.022543
8	1	0	-3.075793	-1.352852	2.266940
9	1	0	-4.294203	-2.142757	0.244769
10	1	0	-3.423791	-1.585440	-2.020666
11	1	0	-1.350690	-0.232895	-2.257928
12	6	0	1.383342	-0.010692	-0.670799
13	1	0	1.090721	-0.810709	-1.356773
14	1	0	2.034793	0.684504	-1.204496
15	6	0	2.108877	-0.591772	0.547677
16	1	0	1.463432	-1.295508	1.079177
17	1	0	2.402963	0.211150	1.227525
18	16	0	3.622734	-1.485419	-0.030196
19	1	0	4.021792	-1.918470	1.183268
20	6	0	0.245470	2.067838	-0.040931
21	6	0	-1.036847	2.803870	0.299115
22	1	0	-1.889092	2.461319	-0.293624
23	1	0	-1.288052	2.660818	1.356271
24	1	0	-0.871610	3.869171	0.126690
25	8	0	1.328521	2.667487	-0.103053
26	7	0	0.166039	0.719557	-0.283572

3



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.98261587 hartree/particle

Thermal correction to Gibbs free energy: 0.169555 hartree/particle

Thermal correction to Enthalpy: 0.22772 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.808661	0.640708	0.404508
2	6	0	4.513493	-0.725710	0.490862
3	6	0	3.228059	-1.192387	0.232978
4	6	0	2.192219	-0.301402	-0.117831
5	6	0	2.489994	1.071703	-0.193162
6	6	0	3.787469	1.527382	0.061178
7	1	0	5.812961	1.003181	0.604704
8	1	0	5.292111	-1.435713	0.759676
9	1	0	3.015436	-2.258497	0.291131
10	1	0	1.717178	1.789988	-0.445820
11	1	0	3.992174	2.593463	-0.004692
12	7	0	0.925007	-0.817576	-0.414475
13	1	0	0.746362	-1.708877	0.035189
14	6	0	-0.251240	0.037547	-0.486069
15	1	0	-0.463625	0.540965	0.471244
16	1	0	-0.076423	0.816258	-1.236165
17	6	0	-1.460840	-0.799551	-0.910291
18	1	0	-1.659362	-1.598148	-0.187772
19	1	0	-1.295076	-1.245627	-1.895267
20	16	0	-2.996170	0.188787	-1.034360
21	6	0	-3.629853	0.017860	0.646111
22	6	0	-4.906237	0.793935	0.896139
23	1	0	-5.382770	1.130188	-0.028736
24	1	0	-5.597267	0.165163	1.466101
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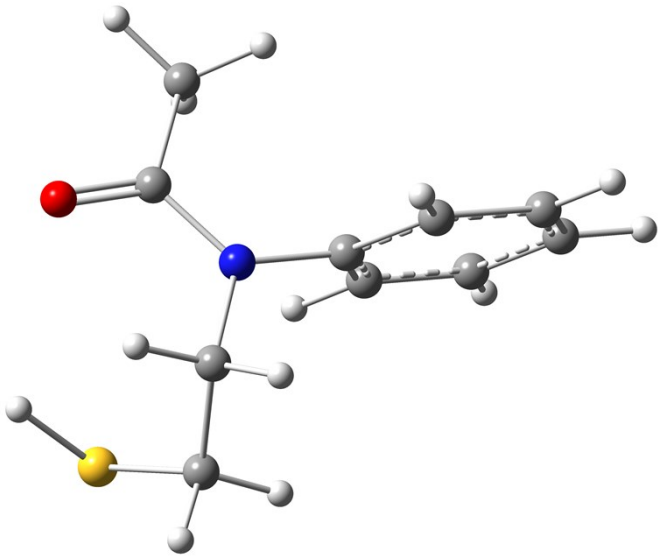
26	8	0	-3.075443	-0.647720	1.495841

without additives

2_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.99262379 hartree/particle

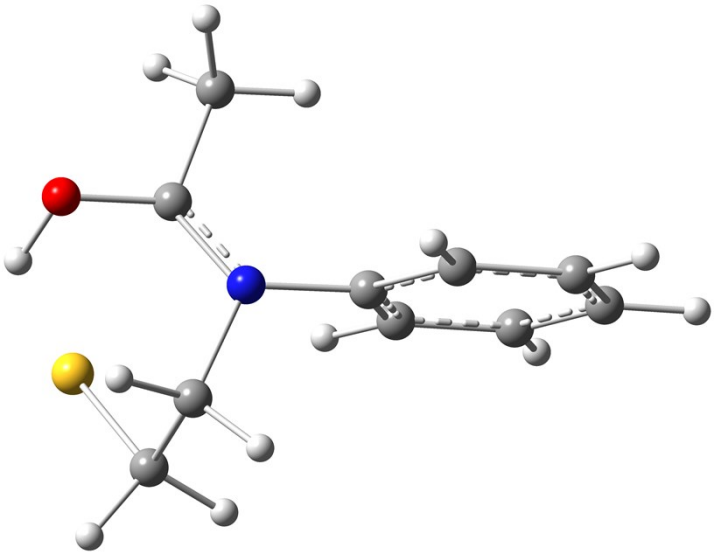
Thermal correction to Gibbs free energy: 0.170630 hartree/particle

Thermal correction to Enthalpy: 0.225952 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.185469	-0.625239	-0.968116
2	6	0	2.500125	-0.990395	-1.272005
3	6	0	3.552925	-0.579688	-0.449585
4	6	0	3.288533	0.200873	0.680338
5	6	0	1.977011	0.573941	0.982908
6	6	0	0.921383	0.166530	0.156444
7	1	0	0.358471	-0.949400	-1.593661
8	1	0	2.699074	-1.601353	-2.148768
9	1	0	4.573982	-0.866948	-0.686528
10	1	0	4.103276	0.524972	1.322699
11	1	0	1.764587	1.190423	1.852830
12	7	0	-0.426678	0.537602	0.487527
13	6	0	-1.113482	-0.243428	1.519998
14	1	0	-0.458131	-0.313835	2.398598
15	1	0	-2.002682	0.324038	1.801594
16	6	0	-1.503685	-1.668541	1.105343
17	1	0	-2.033853	-2.135991	1.942229
18	1	0	-0.614453	-2.274268	0.901321
19	16	0	-2.523611	-1.794170	-0.424525
20	6	0	-1.121480	1.536299	-0.170366
21	6	0	-0.368948	2.330200	-1.224267
22	1	0	-0.941103	3.237033	-1.428020
23	1	0	0.647310	2.590692	-0.914356
24	1	0	-0.292939	1.751031	-2.151877
25	8	0	-2.300062	1.777570	0.087635
26	1	0	-3.321513	-0.734509	-0.171866

ts1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.94898367 hartree/particle

Thermal correction to Gibbs free energy: 0.174706 hartree/particle

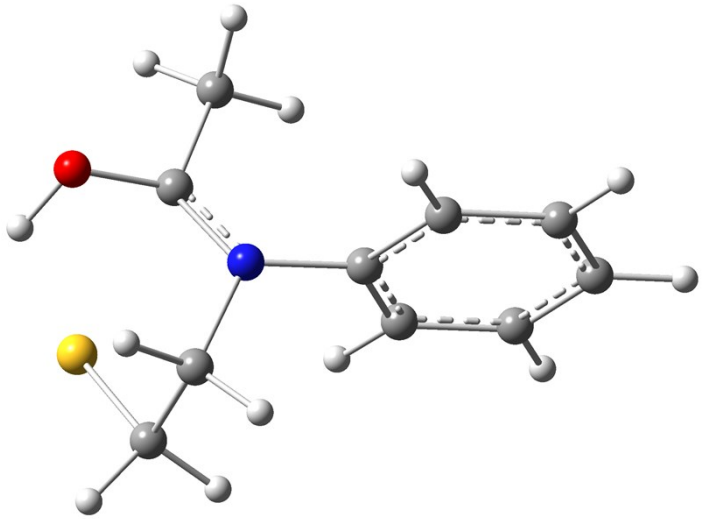
Thermal correction to Enthalpy: 0.225794 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.234104	-0.750806	-0.751185
2	6	0	2.551106	-1.091209	-1.070367
3	6	0	3.619092	-0.513490	-0.376724
4	6	0	3.372292	0.412311	0.641332
5	6	0	2.058874	0.762088	0.966440
6	6	0	0.999837	0.180603	0.265469
7	1	0	0.390106	-1.183574	-1.282867
8	1	0	2.740365	-1.811884	-1.861468
9	1	0	4.641053	-0.784018	-0.628717
10	1	0	4.199349	0.864495	1.181952
11	1	0	1.851020	1.482106	1.753286
12	7	0	-0.355524	0.524294	0.646635
13	6	0	-1.010556	-0.391082	1.600061
14	1	0	-0.260645	-0.694000	2.335940
15	1	0	-1.799708	0.167521	2.107491
16	6	0	-1.602945	-1.618962	0.847556
17	1	0	-2.304067	-2.096050	1.541305
18	1	0	-0.806824	-2.344546	0.642519
19	16	0	-2.456317	-1.164384	-0.704941
20	6	0	-1.151717	1.212392	-0.178307
21	6	0	-0.623126	2.022784	-1.318716
22	1	0	-0.646884	3.079192	-1.017246
23	1	0	0.388889	1.753659	-1.617332
24	1	0	-1.303301	1.911715	-2.166851
25	8	0	-2.381313	1.567827	0.235922
26	1	0	-2.930890	0.725079	0.123870

ts1 optimized in PCM (water)



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d) in PCM (water), 1 atm, 298.15 K

Energy: -916.94853209 hartree/particle

Thermal correction to Gibbs free energy: 0.174256 hartree/particle

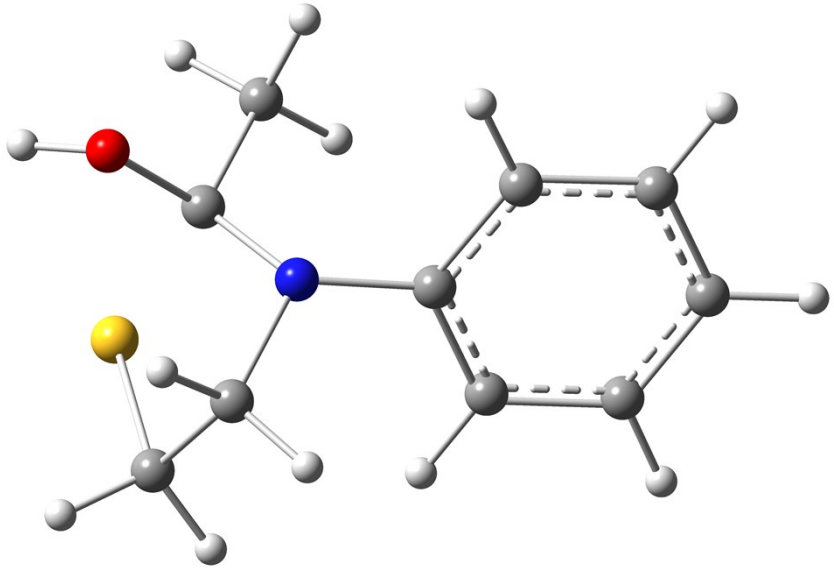
Thermal correction to Enthalpy: 0.226279 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.300839	-0.943035	-0.587924
2	6	0	2.634577	-1.241327	-0.880785
3	6	0	3.667271	-0.480930	-0.322259
4	6	0	3.367061	0.586201	0.530295
5	6	0	2.036031	0.892774	0.827932
6	6	0	1.011447	0.126225	0.266423
7	1	0	0.494597	-1.516221	-1.034254
8	1	0	2.864123	-2.067838	-1.547531
9	1	0	4.702268	-0.718428	-0.552282
10	1	0	4.165392	1.180637	0.965555
11	1	0	1.788508	1.716755	1.490731
12	7	0	-0.355079	0.448822	0.626579
13	6	0	-1.031704	-0.439944	1.582688
14	1	0	-0.288361	-0.810047	2.291510
15	1	0	-1.774479	0.145177	2.128043
16	6	0	-1.716067	-1.611026	0.813538
17	1	0	-2.454506	-2.046759	1.493638
18	1	0	-0.976576	-2.386401	0.590348
19	16	0	-2.527901	-1.048686	-0.731439
20	6	0	-1.140012	1.149960	-0.196927
21	6	0	-0.606520	1.863836	-1.397054
22	1	0	-0.275838	2.865609	-1.088421
23	1	0	0.230381	1.346295	-1.864131
24	1	0	-1.416110	1.990249	-2.118442
25	8	0	-2.285851	1.691157	0.309823
26	1	0	-2.978174	0.992531	0.268055

int1_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.97336682 hartree/particle

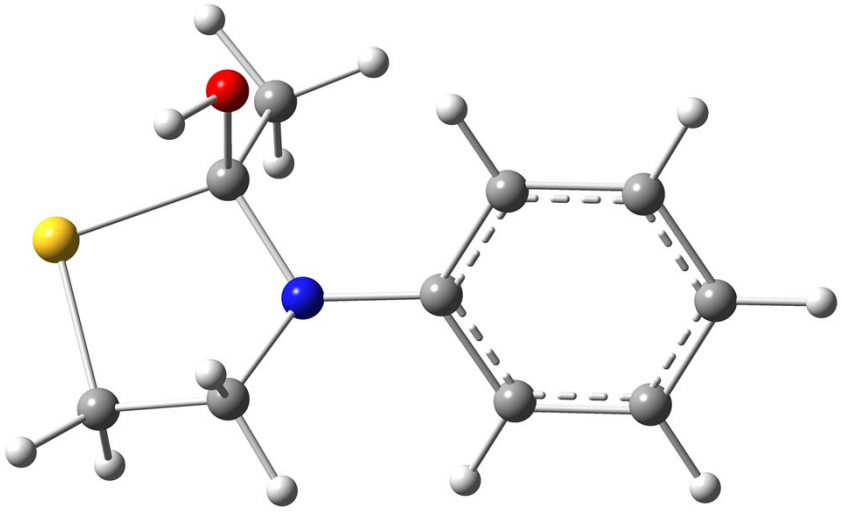
Thermal correction to Gibbs free energy: 0.176680 hartree/particle

Thermal correction to Enthalpy: 0.228077 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.423224	-1.134823	-0.259478
2	6	0	2.757541	-1.317906	-0.633362
3	6	0	3.698315	-0.308813	-0.412286
4	6	0	3.297942	0.883610	0.198607
5	6	0	1.969991	1.060625	0.591085
6	6	0	1.016353	0.058542	0.357644
7	1	0	0.697999	-1.916917	-0.460799
8	1	0	3.057514	-2.248280	-1.109306
9	1	0	4.734264	-0.452134	-0.708151
10	1	0	4.023863	1.670564	0.387574
11	1	0	1.657346	1.968574	1.098555
12	7	0	-0.327992	0.284457	0.798383
13	6	0	-1.026792	-0.803533	1.486576
14	1	0	-0.295288	-1.455078	1.970731
15	1	0	-1.659125	-0.360766	2.261079
16	6	0	-1.928348	-1.584787	0.485593
17	1	0	-2.855444	-1.906087	0.967777
18	1	0	-1.427734	-2.469617	0.080757
19	16	0	-2.290416	-0.426084	-0.895353
20	6	0	-1.259689	0.963893	-0.057564
21	6	0	-0.662684	1.864451	-1.130938
22	1	0	-0.139557	2.702010	-0.659400
23	1	0	0.026390	1.323684	-1.783119
24	1	0	-1.473152	2.274179	-1.742361
25	8	0	-2.122821	1.706942	0.799938
26	1	0	-2.994326	1.764444	0.376217

int1_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.97421990 hartree/particle

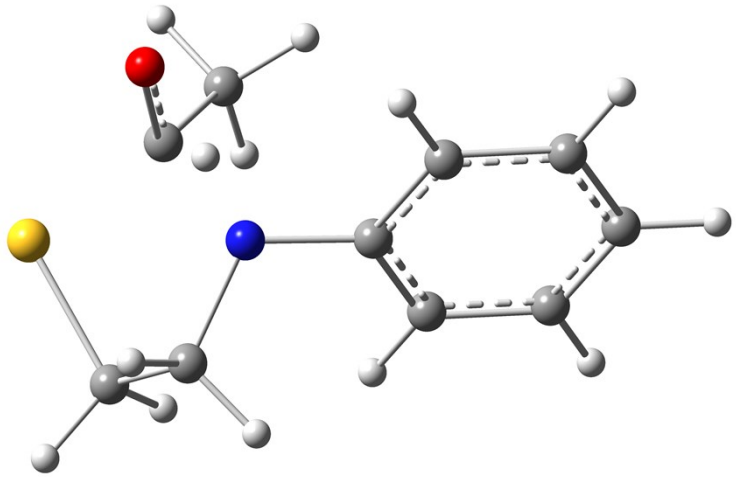
Thermal correction to Gibbs free energy: 0.176349 hartree/particle

Thermal correction to Enthalpy: 0.227868 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.828233	0.852872	-0.391028
2	6	0	-3.225598	0.879098	-0.333752
3	6	0	-3.945901	-0.236630	0.096237
4	6	0	-3.251498	-1.386240	0.488117
5	6	0	-1.857828	-1.410384	0.459504
6	6	0	-1.125459	-0.294983	0.012972
7	1	0	-1.280500	1.715003	-0.752710
8	1	0	-3.750852	1.779160	-0.644601
9	1	0	-5.031923	-0.212338	0.129010
10	1	0	-3.795158	-2.260678	0.837587
11	1	0	-1.323102	-2.292146	0.803502
12	7	0	0.299012	-0.389885	-0.000947
13	6	0	0.918782	-1.366094	-0.898379
14	1	0	0.333361	-2.288982	-0.899047
15	1	0	0.963251	-1.002197	-1.941640
16	6	0	2.324830	-1.592859	-0.350857
17	1	0	3.008983	-1.986803	-1.107191
18	1	0	2.308399	-2.264702	0.512400
19	16	0	2.884411	0.078189	0.170625
20	6	0	1.138822	0.774289	0.226374
21	6	0	0.851694	1.451175	1.563396
22	1	0	-0.146019	1.900190	1.554730
23	1	0	0.908776	0.720460	2.373049
24	1	0	1.581484	2.246074	1.738870
25	8	0	1.036868	1.805131	-0.764407
26	1	0	1.519444	1.523296	-1.558565

ts2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.91735427 hartree/particle

Thermal correction to Gibbs free energy: 0.171634 hartree/particle

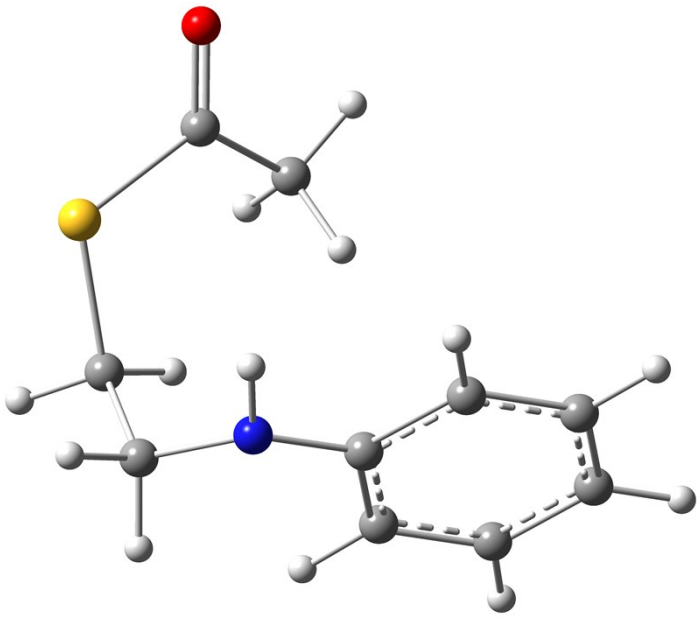
Thermal correction to Enthalpy: 0.222721 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.924147	0.887941	-0.829980
2	6	0	-3.273078	0.826076	-0.471195
3	6	0	-3.738154	-0.208270	0.344262
4	6	0	-2.845567	-1.181521	0.803987
5	6	0	-1.495423	-1.120684	0.454079
6	6	0	-1.031126	-0.084855	-0.367390
7	1	0	-1.559319	1.689298	-1.465856
8	1	0	-3.959177	1.585804	-0.835751
9	1	0	-4.788209	-0.257841	0.619243
10	1	0	-3.198165	-1.988485	1.440947
11	1	0	-0.808168	-1.875391	0.825259
12	7	0	0.362578	0.029535	-0.739217
13	6	0	1.031180	-1.211767	-1.227106
14	1	0	0.276160	-1.969857	-1.455988
15	1	0	1.562107	-0.959064	-2.149768
16	6	0	2.035281	-1.676792	-0.172814
17	1	0	2.755069	-2.380621	-0.602018
18	1	0	1.540910	-2.168434	0.673188
19	16	0	2.912934	-0.163203	0.354265
20	6	0	1.329201	0.922261	0.242705
21	6	0	0.775203	1.187241	1.632672
22	1	0	-0.176732	1.723269	1.563013
23	1	0	0.646634	0.272501	2.218836
24	1	0	1.492649	1.831250	2.151278
25	8	0	1.399321	1.969193	-0.579669
26	1	0	0.696453	1.110737	-1.294064

3_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.98076526 hartree/particle

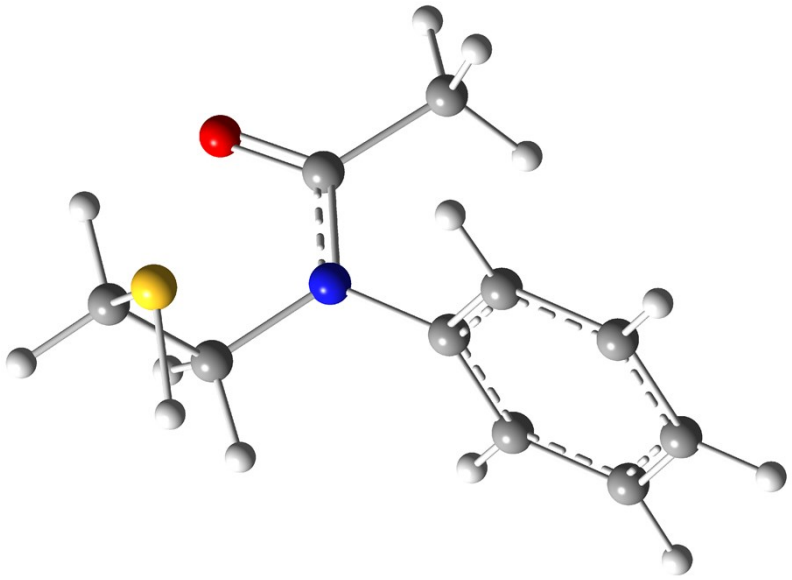
Thermal correction to Gibbs free energy: 0.171552 hartree/particle

Thermal correction to Enthalpy: 0.227684 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.083859	0.660310	-1.029702
2	6	0	-3.260868	0.832690	-0.306185
3	6	0	-3.686720	-0.136679	0.609940
4	6	0	-2.907200	-1.281606	0.784082
5	6	0	-1.722484	-1.466042	0.065129
6	6	0	-1.291977	-0.495821	-0.861416
7	1	0	-1.769453	1.421323	-1.741728
8	1	0	-3.849495	1.733977	-0.459574
9	1	0	-4.604504	-0.000025	1.174416
10	1	0	-3.217745	-2.048689	1.489674
11	1	0	-1.145713	-2.372139	0.222693
12	7	0	-0.147035	-0.654622	-1.642848
13	6	0	0.928475	-1.568847	-1.312772
14	1	0	0.515250	-2.573509	-1.159294
15	1	0	1.578834	-1.636863	-2.191370
16	6	0	1.773689	-1.193943	-0.077740
17	1	0	2.512194	-1.980805	0.113719
18	1	0	1.147158	-1.107304	0.812125
19	16	0	2.724277	0.366672	-0.326056
20	6	0	2.013663	1.641569	0.752766
21	6	0	0.931723	1.289531	1.750944
22	1	0	0.683629	2.197218	2.306174
23	1	0	0.032467	0.912953	1.252393
24	1	0	1.279712	0.522085	2.451726
25	8	0	2.474855	2.756399	0.637782
26	1	0	0.160480	0.191028	-2.107037

2_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.99090264 hartree/particle

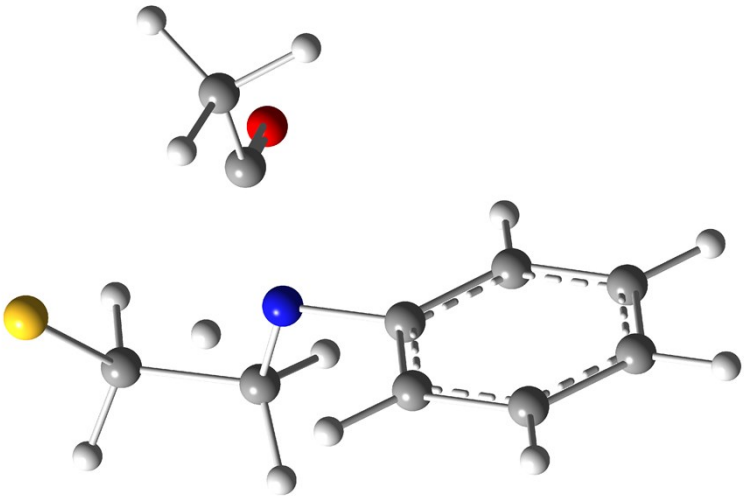
Thermal correction to Gibbs free energy: 0.169799 hartree/particle

Thermal correction to Enthalpy: 0.225847 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.327247	-0.712827	1.012105
2	6	0	-2.656493	-1.089522	1.222856
3	6	0	-3.661330	-0.643683	0.359445
4	6	0	-3.333393	0.184635	-0.718127
5	6	0	-2.007027	0.571504	-0.925320
6	6	0	-0.999472	0.124731	-0.059625
7	1	0	-0.536647	-1.079154	1.659242
8	1	0	-2.904210	-1.739546	2.058126
9	1	0	-4.693638	-0.941497	0.523574
10	1	0	-4.109389	0.536583	-1.393062
11	1	0	-1.747008	1.226097	-1.753627
12	6	0	1.114578	-0.104645	-1.389099
13	1	0	0.402678	-0.690358	-1.977650
14	1	0	1.518710	0.689896	-2.029293
15	6	0	2.296509	-0.978680	-0.951912
16	1	0	2.975180	-0.388913	-0.331765
17	1	0	2.852134	-1.293180	-1.841929
18	16	0	1.883595	-2.460685	0.057770
19	6	0	0.957061	1.584140	0.363657
20	6	0	0.156716	2.284202	1.448773
21	1	0	-0.851714	2.549347	1.116053
22	1	0	0.050819	1.641365	2.330175
23	1	0	0.701861	3.185747	1.733366
24	8	0	2.099157	1.941218	0.074550
25	1	0	1.150974	-3.103562	-0.879541
26	7	0	0.364481	0.521769	-0.289580

ts3



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.94273535 hartree/particle

Thermal correction to Gibbs free energy: 0.175404 hartree/particle

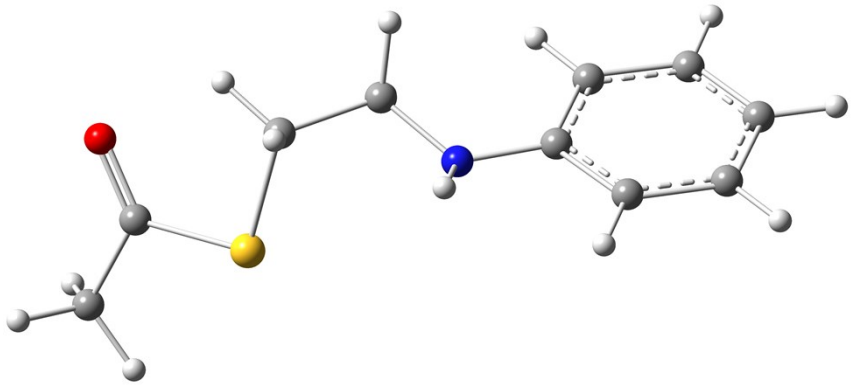
Thermal correction to Enthalpy: 0.226746 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.707005	-1.178552	0.690448
2	6	0	-3.102490	-1.213798	0.745998
3	6	0	-3.856791	-0.266661	0.048597
4	6	0	-3.214188	0.718502	-0.708090
5	6	0	-1.819959	0.761543	-0.774209
6	6	0	-1.077930	-0.191540	-0.071308
7	1	0	-1.113003	-1.912959	1.228711
8	1	0	-3.596078	-1.981057	1.335766
9	1	0	-4.941869	-0.295242	0.094204
10	1	0	-3.797696	1.456967	-1.250754
11	1	0	-1.315910	1.525947	-1.357833
12	6	0	1.006078	-0.675452	-1.397263
13	1	0	0.560856	-1.660939	-1.562102
14	1	0	0.717916	-0.000862	-2.205284
15	6	0	2.537132	-0.744557	-1.185104
16	1	0	2.996696	0.158155	-1.598725
17	1	0	2.924500	-1.605787	-1.739074
18	16	0	2.951448	-0.871952	0.601546
19	6	0	1.021768	1.198828	0.284575
20	6	0	0.866878	1.536966	1.741391
21	1	0	-0.057914	2.117315	1.872975
22	1	0	0.836933	0.649790	2.375373
23	1	0	1.710921	2.162267	2.038358
24	8	0	1.299332	1.957430	-0.610616
25	1	0	0.852790	-0.806681	0.594524
26	7	0	0.383295	-0.169545	-0.116594

3_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -916.98203739 hartree/particle

Thermal correction to Gibbs free energy: 0.169531 hartree/particle

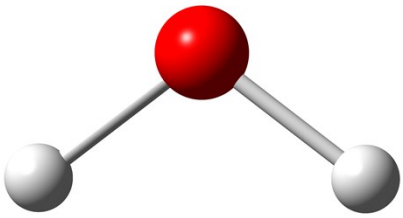
Thermal correction to Enthalpy: 0.227644 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.789890	-1.991897	0.184929
2	6	0	-4.171476	-2.031095	0.023064
3	6	0	-4.833647	-1.039693	-0.712066
4	6	0	-4.081353	-0.012924	-1.283784
5	6	0	-2.691961	0.034978	-1.133126
6	6	0	-2.024240	-0.955004	-0.388384
7	1	0	-2.289324	-2.762149	0.769298
8	1	0	-4.736315	-2.842181	0.476595
9	1	0	-5.912315	-1.071404	-0.836476
10	1	0	-4.573998	0.764839	-1.862661
11	1	0	-2.137075	0.844018	-1.596552
12	6	0	0.243121	-0.089257	-0.958517
13	1	0	0.184451	-0.326368	-2.036933
14	1	0	-0.055180	0.958088	-0.839745
15	6	0	1.694044	-0.247061	-0.514276
16	1	0	2.357761	0.344744	-1.152530
17	1	0	2.011095	-1.294768	-0.573671
18	16	0	1.988697	0.338759	1.201543
19	6	0	3.288667	1.555060	0.912859
20	6	0	3.784326	2.214086	2.184054
21	1	0	3.754141	3.300694	2.051592
22	1	0	3.197845	1.933081	3.062806
23	1	0	4.829816	1.924494	2.341223
24	8	0	3.731275	1.821007	-0.186051
25	1	0	-0.255340	-1.834869	0.060622
26	7	0	-0.644057	-0.927129	-0.168297

with H_2O

H_2O



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -76.42874237 hartree/particle

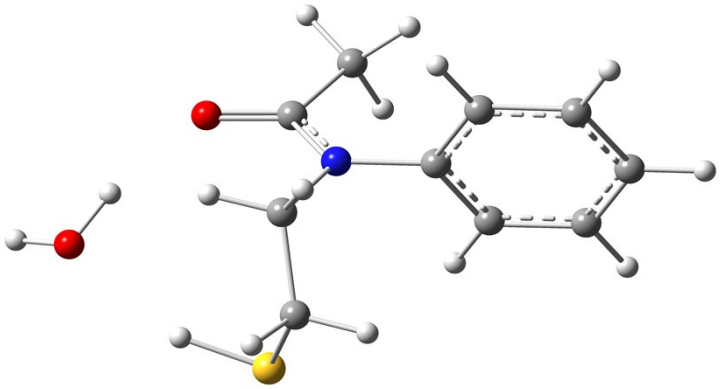
Thermal correction to Gibbs free energy: 0.003434 hartree/particle

Thermal correction to Enthalpy: 0.024874 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.117291
2	1	0	0.000000	-0.771299	-0.469165
3	1	0	0.000000	0.771299	-0.469165

2·H_2O_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.43270547 hartree/particle

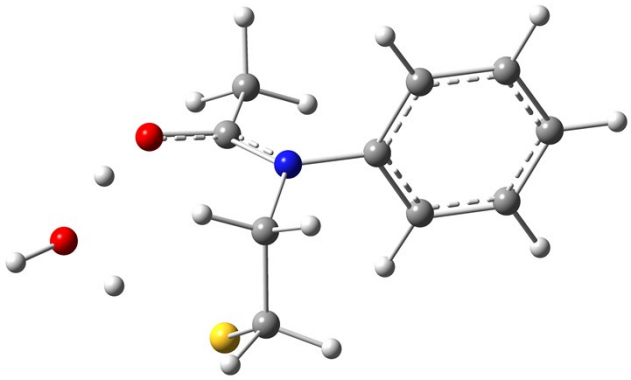
Thermal correction to Gibbs free energy: 0.192556 hartree/particle

Thermal correction to Enthalpy: 0.253858 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.621989	0.603256	-0.935365
2	6	0	-2.966027	0.931930	-1.133711
3	6	0	-3.948591	0.425753	-0.278292
4	6	0	-3.584834	-0.413969	0.779257
5	6	0	-2.243772	-0.751048	0.976584
6	6	0	-1.260566	-0.248107	0.115221
7	1	0	-0.848061	1.004803	-1.583339
8	1	0	-3.242437	1.590468	-1.953032
9	1	0	-4.992471	0.685708	-0.432817
10	1	0	-4.344503	-0.811232	1.447397
11	1	0	-1.953897	-1.411170	1.790270
12	7	0	0.120995	-0.583218	0.340209
13	6	0	0.819908	0.145685	1.409004
14	1	0	0.244400	0.026755	2.337769
15	1	0	1.787060	-0.335366	1.552194
16	6	0	0.999752	1.648388	1.152757
17	1	0	1.523134	2.077207	2.013862
18	1	0	0.027991	2.147609	1.081530
19	16	0	1.885743	2.101571	-0.393879
20	6	0	0.784941	-1.518432	-0.412597
21	6	0	-0.001025	-2.248634	-1.486405
22	1	0	-1.007166	-2.528307	-1.162648
23	1	0	-0.103129	-1.613019	-2.373664
24	1	0	0.564241	-3.140256	-1.763134
25	8	0	1.981681	-1.782062	-0.237593
26	1	0	3.507827	-0.896884	0.217556
27	8	0	4.188946	-0.247580	0.500041
28	1	0	3.013301	1.389491	-0.140696
29	1	0	5.027804	-0.550050	0.123512

ts4·H_2O



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.39782131 hartree/particle

Thermal correction to Gibbs free energy: 0.193431 hartree/particle

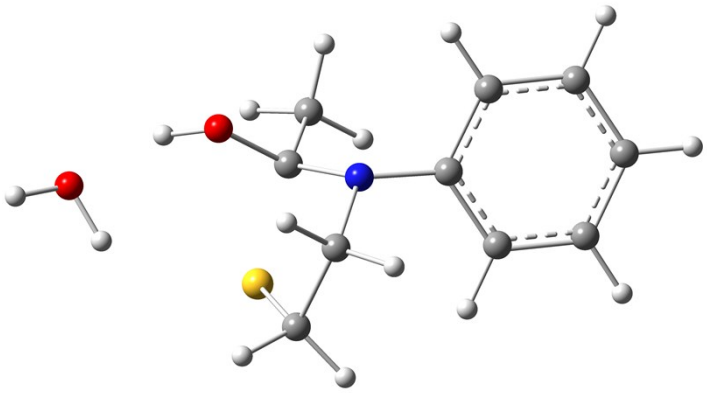
Thermal correction to Enthalpy: 0.250346 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.596027	0.862851	-0.625895
2	6	0	-2.917970	1.131089	-0.991204
3	6	0	-3.966142	0.358125	-0.482156
4	6	0	-3.695017	-0.693605	0.397914
5	6	0	-2.376990	-0.970463	0.770724
6	6	0	-1.336475	-0.192950	0.254318
7	1	0	-0.764335	1.437334	-1.027895
8	1	0	-3.126015	1.947207	-1.678054
9	1	0	-4.991527	0.574404	-0.770408
10	1	0	-4.505951	-1.297203	0.796621
11	1	0	-2.151583	-1.780623	1.459256
12	7	0	0.015937	-0.477177	0.682325
13	6	0	0.619754	0.420370	1.690841
14	1	0	-0.144206	0.625994	2.447126
15	1	0	1.437322	-0.128775	2.156186
16	6	0	1.135571	1.749855	1.061777
17	1	0	1.816489	2.184810	1.803595
18	1	0	0.292856	2.444255	0.968557
19	16	0	1.949239	1.642685	-0.581815
20	6	0	0.825073	-1.268900	-0.015304
21	6	0	0.404039	-1.922366	-1.299210
22	1	0	0.052682	-2.940104	-1.082956
23	1	0	-0.381249	-1.375628	-1.819653
24	1	0	1.283082	-2.006468	-1.943613
25	8	0	1.955818	-1.619547	0.520364
26	1	0	2.872305	-1.316555	-0.028201
27	8	0	3.852890	-0.620952	-0.608763
28	1	0	3.330782	0.301364	-0.571563
29	1	0	4.635396	-0.532776	-0.039870

int2·H_2O_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.41215574 hartree/particle

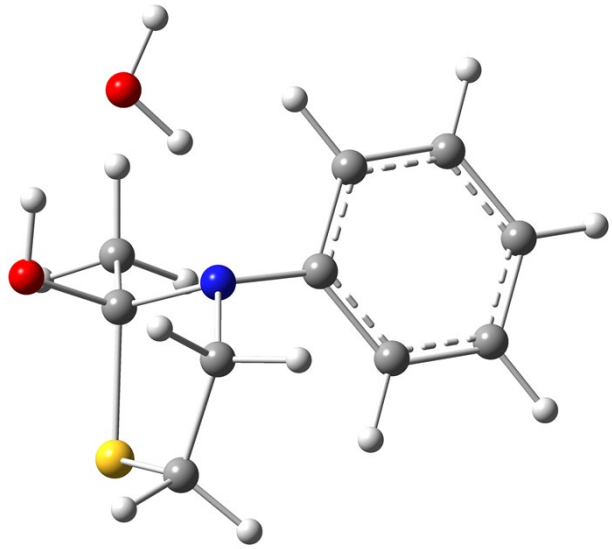
Thermal correction to Gibbs free energy: 0.197601 hartree/particle

Thermal correction to Enthalpy: 0.255876 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893146	1.160100	-0.202716
2	6	0	-3.206313	1.273091	-0.668036
3	6	0	-4.062459	0.169247	-0.643511
4	6	0	-3.599574	-1.049514	-0.137652
5	6	0	-2.294756	-1.159303	0.345974
6	6	0	-1.424541	-0.059401	0.310016
7	1	0	-1.230433	2.017962	-0.253186
8	1	0	-3.554867	2.224831	-1.061520
9	1	0	-5.081855	0.259020	-1.009684
10	1	0	-4.260527	-1.911987	-0.101798
11	1	0	-1.937597	-2.092051	0.772650
12	7	0	-0.103278	-0.222509	0.838807
13	6	0	0.437597	0.835555	1.693574
14	1	0	-0.386243	1.355587	2.188280
15	1	0	1.058731	0.365107	2.459796
16	6	0	1.322122	1.815019	0.858672
17	1	0	2.199316	2.126520	1.432130
18	1	0	0.772667	2.713188	0.561035
19	16	0	1.822776	0.909170	-0.659027
20	6	0	0.944615	-0.726866	-0.000490
21	6	0	0.525047	-1.556387	-1.206401
22	1	0	0.056712	-2.485221	-0.865422
23	1	0	-0.165700	-1.017621	-1.858304
24	1	0	1.417927	-1.820491	-1.781857
25	8	0	1.834275	-1.420140	0.830790
26	1	0	2.694141	-1.542769	0.371657
27	8	0	4.303899	-1.177173	-0.522805
28	1	0	4.008114	-0.249075	-0.626211
29	1	0	5.115151	-1.150201	0.006774

int2·H_2O_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.41461066 hartree/particle

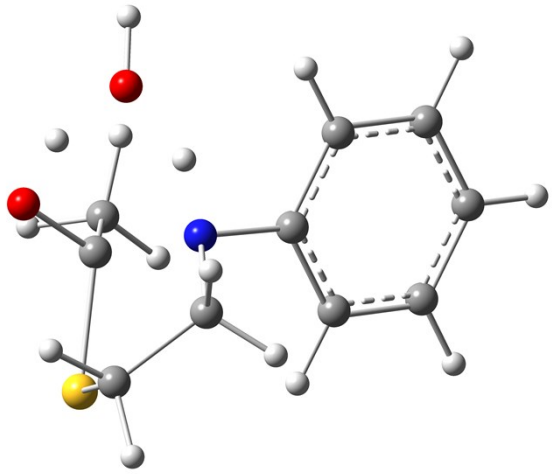
Thermal correction to Gibbs free energy: 0.198285 hartree/particle

Thermal correction to Enthalpy: 0.25583 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.930770	1.014647	0.193628
2	6	0	-3.284642	0.707402	0.338211
3	6	0	-3.755653	-0.565043	0.003192
4	6	0	-2.857300	-1.525161	-0.467752
5	6	0	-1.498785	-1.223254	-0.596847
6	6	0	-1.018976	0.053471	-0.268430
7	1	0	-1.572292	2.009062	0.444071
8	1	0	-3.972063	1.467504	0.700694
9	1	0	-4.810666	-0.804495	0.105832
10	1	0	-3.209333	-2.520227	-0.727874
11	1	0	-0.815275	-1.990591	-0.941709
12	7	0	0.366394	0.437320	-0.412476
13	6	0	1.083152	-0.123941	-1.579711
14	1	0	0.374233	-0.261943	-2.399612
15	1	0	1.829037	0.610466	-1.891441
16	6	0	1.811953	-1.447181	-1.205795
17	1	0	2.818000	-1.461085	-1.632667
18	1	0	1.276883	-2.333306	-1.561162
19	16	0	1.894484	-1.501210	0.628479
20	6	0	1.255661	0.251246	0.763753
21	6	0	0.588699	0.464503	2.118604
22	1	0	0.240969	1.500036	2.206906
23	1	0	-0.253472	-0.210956	2.282193
24	1	0	1.339715	0.294792	2.895090
25	1	0	0.476934	2.387727	-0.722522
26	1	0	2.074047	2.012585	0.489998
27	8	0	2.382451	1.090201	0.615370
28	8	0	0.961704	3.236625	-0.598232
29	1	0	0.305801	3.949030	-0.595699

ts5·H_2O



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.38414345 hartree/particle

Thermal correction to Gibbs free energy: 0.195081 hartree/particle

Thermal correction to Enthalpy: 0.249531 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.981355	1.163886	-0.153114
2	6	0	-3.346144	0.919082	0.022948
3	6	0	-3.822093	-0.392063	0.086942
4	6	0	-2.926715	-1.460450	-0.028260
5	6	0	-1.562541	-1.224275	-0.206279
6	6	0	-1.090699	0.092304	-0.265237
7	1	0	-1.608670	2.182086	-0.213251
8	1	0	-4.034043	1.756271	0.104796
9	1	0	-4.883443	-0.582008	0.221961
10	1	0	-3.289355	-2.483691	0.022278
11	1	0	-0.865211	-2.053142	-0.278502
12	7	0	0.326882	0.390683	-0.444565
13	6	0	0.938789	-0.224432	-1.686424
14	1	0	0.210846	-0.915661	-2.112599
15	1	0	1.118845	0.586089	-2.398552
16	6	0	2.237764	-0.959511	-1.323125
17	1	0	3.097921	-0.287127	-1.337073
18	1	0	2.417902	-1.796705	-2.002229
19	16	0	1.992049	-1.581486	0.376455
20	6	0	1.311789	0.104051	0.812053
21	6	0	0.549175	0.077245	2.131357
22	1	0	0.066327	1.046352	2.298126
23	1	0	-0.199328	-0.716164	2.188522
24	1	0	1.289150	-0.067519	2.923806
25	1	0	0.464401	1.523590	-0.548442
26	1	0	1.902313	1.973188	0.257452
27	8	0	2.275272	1.045421	0.765545
28	8	0	1.163817	2.744064	-0.551479
29	1	0	0.790861	3.512539	-0.095307

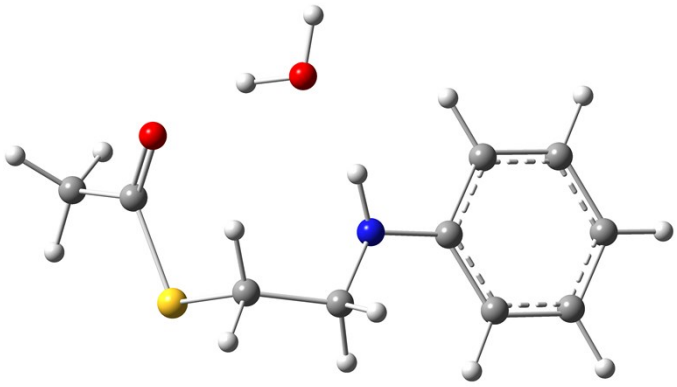
NBO analysis of **ts5·H_2O** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
49. LP (1) N 12	/ 52. LP*(1) H 25	327.09	0.50	0.374
49. LP (1) N 12	/328. RY*(1) H 25	3.47	2.90	0.099
49. LP (1) N 12	/329. RY*(2) H 25	1.21	1.58	0.043
49. LP (1) N 12	/330. RY*(3) H 25	0.10	2.82	0.016
49. LP (1) N 12	/332. RY*(5) H 25	0.20	2.29	0.021
from unit 4 to unit 3				
57. LP (1) O 28	/ 53. LP*(1) H 26	3.91	0.69	0.053
57. LP (1) O 28	/333. RY*(1) H 26	0.72	2.72	0.040
57. LP (1) O 28	/335. RY*(3) H 26	0.15	2.23	0.016
58. LP (2) O 28	/ 53. LP*(1) H 26	23.17	0.49	0.104
58. LP (2) O 28	/334. RY*(2) H 26	0.42	2.81	0.032
58. LP (2) O 28	/336. RY*(4) H 26	0.07	2.36	0.012
58. LP (2) O 28	/337. RY*(5) H 26	0.13	1.58	0.013
59. LP (3) O 28	/ 53. LP*(1) H 26	117.04	0.78	0.290
59. LP (3) O 28	/333. RY*(1) H 26	0.72	2.81	0.042
59. LP (3) O 28	/334. RY*(2) H 26	0.81	3.10	0.047
59. LP (3) O 28	/336. RY*(4) H 26	0.30	2.66	0.027
59. LP (3) O 28	/337. RY*(5) H 26	0.22	1.87	0.019

3·H_2O_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.42144847 hartree/particle

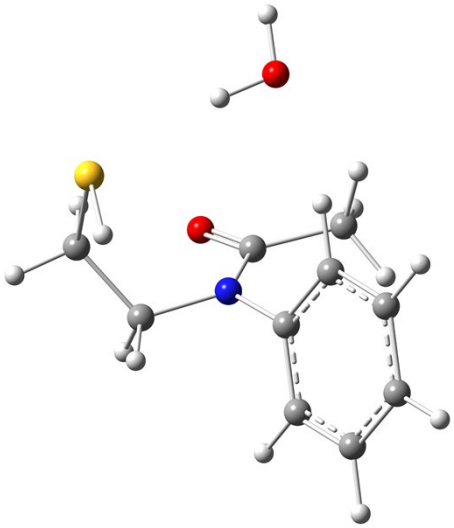
Thermal correction to Gibbs free energy: 0.191080 hartree/particle

Thermal correction to Enthalpy: 0.255393 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.581206	1.075948	-0.361165
2	6	0	-3.968880	0.984928	-0.392237
3	6	0	-4.601424	-0.179240	-0.848107
4	6	0	-3.809723	-1.244834	-1.277620
5	6	0	-2.413643	-1.163973	-1.257413
6	6	0	-1.771652	-0.001049	-0.787544
7	1	0	-2.101637	1.981758	0.003427
8	1	0	-4.563654	1.831555	-0.056392
9	1	0	-5.685395	-0.248569	-0.871122
10	1	0	-4.277134	-2.156244	-1.643935
11	1	0	-1.835290	-2.010221	-1.613384
12	7	0	-0.386224	0.128427	-0.689570
13	6	0	0.519651	-0.786035	-1.350955
14	1	0	0.202740	-1.815469	-1.153937
15	1	0	0.521673	-0.657224	-2.449941
16	6	0	1.962896	-0.610207	-0.865371
17	1	0	2.283884	0.433920	-0.915850
18	1	0	2.635868	-1.202326	-1.493059
19	16	0	2.232405	-1.191648	0.856826
20	6	0	2.495521	0.309698	1.776669
21	6	0	2.706171	0.076449	3.258289
22	1	0	1.845087	0.488967	3.797274
23	1	0	2.810154	-0.981883	3.510781
24	1	0	3.598035	0.624690	3.578942
25	1	0	-0.065038	1.096028	-0.700175
26	1	0	1.633148	2.524700	0.039881
27	8	0	2.512987	1.430835	1.291335
28	8	0	1.057101	2.775250	-0.709156
29	1	0	0.878947	3.722635	-0.622017

2_H_2O_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.42536118 hartree/particle

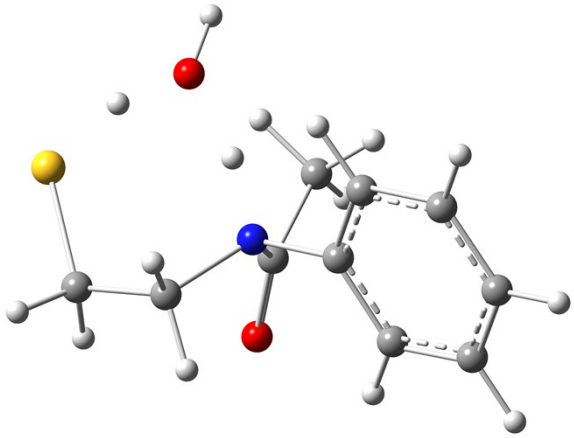
Thermal correction to Gibbs free energy: 0.189581 hartree/particle

Thermal correction to Enthalpy: 0.253298 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.110817	-0.972654	-0.844209
2	6	0	-3.438417	-0.540859	-0.877418
3	6	0	-3.812692	0.627229	-0.206301
4	6	0	-2.849239	1.360558	0.491132
5	6	0	-1.515261	0.942540	0.515618
6	6	0	-1.142662	-0.230734	-0.150970
7	1	0	-1.822983	-1.891736	-1.348699
8	1	0	-4.180368	-1.124085	-1.417000
9	1	0	-4.846759	0.961309	-0.226373
10	1	0	-3.130103	2.270584	1.015212
11	1	0	-0.770469	1.519929	1.053757
12	6	0	0.911415	-0.823082	-1.441757
13	1	0	1.174026	-1.877937	-1.599357
14	1	0	0.200038	-0.530622	-2.218517
15	6	0	2.211268	-0.024938	-1.604995
16	1	0	2.609797	-0.222780	-2.605611
17	1	0	2.947558	-0.359780	-0.872358
18	16	0	2.102557	1.799205	-1.368286
19	6	0	0.844739	-1.230987	0.959398
20	6	0	0.119857	-1.181792	2.289241
21	1	0	0.623415	-1.876695	2.964011
22	1	0	0.186358	-0.171117	2.707576
23	1	0	-0.938658	-1.444585	2.205199
24	8	0	1.964483	-1.733029	0.855184
25	7	0	0.224274	-0.681274	-0.150068
26	8	0	1.166712	2.313775	1.891514
27	1	0	1.873680	2.739431	2.399077
28	1	0	0.995115	2.021375	-2.110107
29	1	0	1.519667	2.199160	0.986880

ts6·H_2O



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.37630302 hartree/particle

Thermal correction to Gibbs free energy: 0.190641 hartree/particle

Thermal correction to Enthalpy: 0.247783 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.059076	-1.054119	-0.402063
2	6	0	-3.447005	-0.903383	-0.453281
3	6	0	-4.031742	0.342072	-0.207610
4	6	0	-3.224443	1.443296	0.088572
5	6	0	-1.835110	1.306285	0.147451
6	6	0	-1.263686	0.053490	-0.093826
7	1	0	-1.605559	-2.019956	-0.601005
8	1	0	-4.068736	-1.762722	-0.688712
9	1	0	-5.111724	0.453880	-0.250157
10	1	0	-3.672357	2.415690	0.274101
11	1	0	-1.195535	2.155822	0.367919
12	6	0	0.822344	0.002999	-1.443774
13	1	0	0.293516	-0.717221	-2.074949
14	1	0	0.581963	1.013847	-1.784478
15	6	0	2.334127	-0.254108	-1.491928
16	1	0	2.658298	0.100122	-2.478044
17	1	0	2.519892	-1.330595	-1.459146
18	16	0	3.365387	0.534474	-0.179826
19	6	0	0.629001	-1.283627	0.721337
20	6	0	0.715018	-1.071731	2.205900
21	1	0	1.616168	-0.485753	2.418492
22	1	0	-0.154285	-0.518185	2.577721
23	1	0	0.786722	-2.040303	2.703610
24	8	0	0.819591	-2.317323	0.136003
25	7	0	0.210884	-0.064138	-0.050375
26	8	0	1.183377	2.109344	0.769471
27	1	0	1.312806	2.307972	1.711104
28	1	0	2.250298	1.600247	0.359093
29	1	0	0.605847	0.901324	0.485821

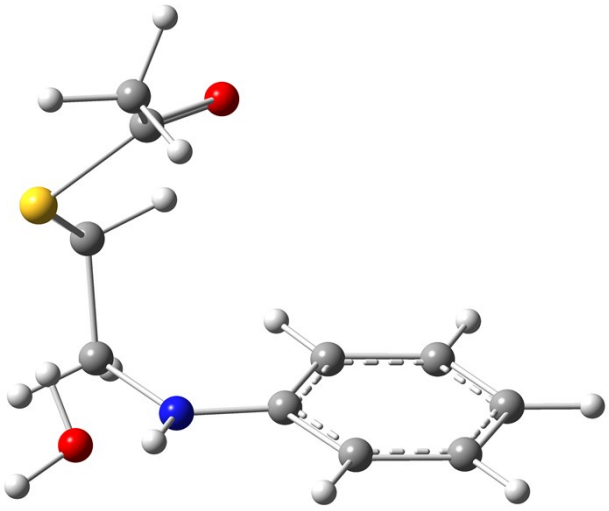
NBO analysis of **ts6·H_2O** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 3				
54. LP (1) N 25	/ 58. LP*(1) H 29	291.17	0.51	0.359
54. LP (1) N 25	/371. RY*(1) H 29	2.98	2.96	0.092
54. LP (1) N 25	/372. RY*(2) H 29	1.93	1.29	0.049
from unit 2 to unit 1				
55. LP (1) O 26	/366. RY*(1) H 28	0.37	2.27	0.026
55. LP (1) O 26	/367. RY*(2) H 28	0.47	2.11	0.028
55. LP (1) O 26	/368. RY*(3) H 28	0.14	2.74	0.017
55. LP (1) O 26	/369. RY*(4) H 28	0.21	2.11	0.019
55. LP (1) O 26	/370. RY*(5) H 28	0.12	2.02	0.014

3·H_2O_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -993.41890647 hartree/particle

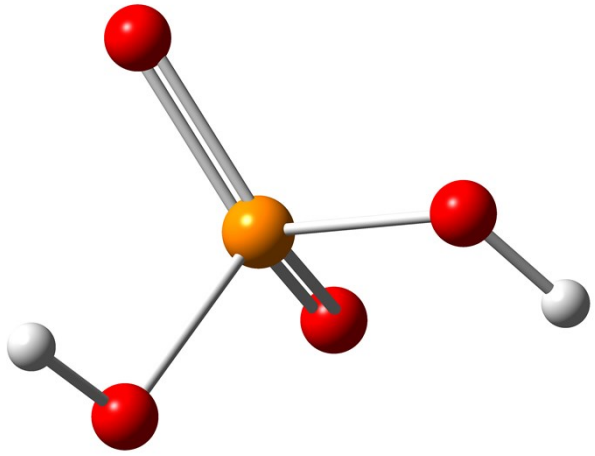
Thermal correction to Gibbs free energy: 0.188893 hartree/particle

Thermal correction to Enthalpy: 0.254956 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.000788	0.300586	-1.563197
2	6	0	3.329674	-0.108559	-1.515778
3	6	0	4.105943	0.100841	-0.368576
4	6	0	3.517445	0.727735	0.730819
5	6	0	2.183274	1.142835	0.698354
6	6	0	1.400612	0.941898	-0.456458
7	1	0	1.409261	0.133621	-2.461023
8	1	0	3.763793	-0.598112	-2.384747
9	1	0	5.142594	-0.222100	-0.333848
10	1	0	4.097191	0.895554	1.635752
11	1	0	1.759764	1.620586	1.576454
12	7	0	0.085944	1.373939	-0.563140
13	6	0	-0.701619	1.892839	0.526117
14	1	0	-0.120440	2.643654	1.079818
15	1	0	-1.553550	2.429642	0.093253
16	6	0	-1.206328	0.859596	1.558547
17	1	0	-1.666549	1.374635	2.408687
18	1	0	-0.391732	0.230225	1.930773
19	16	0	-2.462844	-0.299275	0.882695
20	6	0	-1.670578	-1.911344	1.169150
21	8	0	-0.635873	-2.033590	1.781196
22	1	0	-2.421318	-0.023973	-1.663921
23	1	0	-0.425329	1.083282	-1.389873
24	6	0	-2.432255	-3.067855	0.558063
25	1	0	-3.488780	-2.833280	0.399373
26	1	0	-1.977998	-3.307413	-0.411428
27	1	0	-2.333824	-3.942497	1.207226
28	8	0	-1.973439	0.271486	-2.477747
29	1	0	-2.661497	0.643078	-3.049853

$H_2PO_4^-$



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -643.70849982 hartree/particle

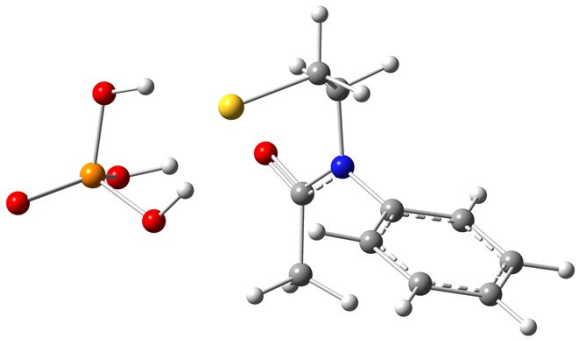
Thermal correction to Gibbs free energy: 0.007783 hartree/particle

Thermal correction to Enthalpy: 0.043145 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000017	0.000248	0.175623
2	8	0	-0.994052	0.834419	-0.896105
3	1	0	-1.773986	0.272313	-1.025711
4	8	0	0.994392	-0.836854	-0.893568
5	1	0	1.774334	-0.275133	-1.024667
6	8	0	0.871425	1.024005	0.857136
7	8	0	-0.871777	-1.021683	0.859542

2·$H_2PO_4^-$_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.71942067 hartree/particle

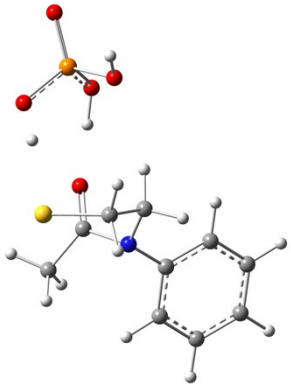
Thermal correction to Gibbs free energy: 0.202788 hartree/particle

Thermal correction to Enthalpy: 0.272288 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.437360	0.720896	0.868289
2	6	0	3.660405	0.989944	1.489392
3	6	0	4.834085	0.373293	1.045187
4	6	0	4.785961	-0.514400	-0.034621
5	6	0	3.566601	-0.785126	-0.660838
6	6	0	2.388946	-0.178833	-0.202935
7	1	0	1.518890	1.213483	1.180888
8	1	0	3.692883	1.688919	2.321825
9	1	0	5.782148	0.585569	1.534510
10	1	0	5.694952	-0.994967	-0.389629
11	1	0	3.515417	-1.474050	-1.500691
12	7	0	1.144542	-0.463987	-0.863228
13	6	0	0.729142	0.436576	-1.960107
14	1	0	1.462481	0.335030	-2.777915
15	1	0	-0.230074	0.056481	-2.312213
16	6	0	0.613217	1.915849	-1.572275
17	1	0	0.340635	2.444110	-2.496088
18	1	0	1.601308	2.297512	-1.282753
19	16	0	-0.601111	2.354634	-0.256127
20	6	0	0.373436	-1.548671	-0.550063
21	6	0	0.720697	-2.355745	0.685773
22	1	0	1.782609	-2.352819	0.939511
23	1	0	0.158337	-1.924135	1.523067
24	1	0	0.372448	-3.380297	0.534490
25	8	0	-0.623498	-1.852179	-1.225975
26	1	0	-2.238974	-1.862791	-0.434612
27	8	0	-3.054187	-1.772262	0.114657
28	15	0	-3.183770	-0.311094	0.795003
29	8	0	-1.719006	-0.024216	1.426424
30	8	0	-3.310614	0.739900	-0.421085
31	8	0	-4.311283	-0.297712	1.759714
32	1	0	-1.209622	0.708671	0.949975
33	1	0	-2.492980	1.310339	-0.565141

ts4·$H_2PO_4^-$



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.68106238 hartree/particle

Thermal correction to Gibbs free energy: 0.200445 hartree/particle

Thermal correction to Enthalpy: 0.269604 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.733385	0.573370	-0.182358
2	6	0	-4.969946	-0.059304	-0.315642
3	6	0	-5.102723	-1.427615	-0.056012
4	6	0	-3.973309	-2.154493	0.330996
5	6	0	-2.728799	-1.530808	0.444955
6	6	0	-2.585210	-0.151341	0.193966
7	1	0	-3.651062	1.643314	-0.340857
8	1	0	-5.840110	0.527704	-0.603275
9	1	0	-6.069587	-1.916552	-0.149934
10	1	0	-4.053622	-3.221438	0.529937
11	1	0	-1.855681	-2.116579	0.714570
12	7	0	-1.333353	0.506017	0.332873
13	6	0	-0.399216	0.019613	1.358887
14	1	0	-0.988113	-0.466717	2.145780
15	1	0	0.305661	-0.720535	0.960117
16	6	0	0.359170	1.220853	1.942447
17	1	0	1.163236	0.844563	2.586845
18	1	0	-0.330531	1.805537	2.564687
19	16	0	1.039598	2.307121	0.628172
20	6	0	-0.682555	0.881119	-0.915642
21	6	0	-1.288865	2.034069	-1.688209
22	1	0	-2.114072	1.657955	-2.311772
23	1	0	-1.655218	2.817555	-1.023587
24	1	0	-0.524292	2.443205	-2.351712
25	8	0	0.081828	0.092892	-1.488307
26	1	0	1.448235	-0.872446	-1.182997
27	8	0	2.237640	-1.467671	-1.068526
28	15	0	3.481068	-0.858054	-0.272271
29	8	0	3.440964	0.722947	-0.401423
30	8	0	3.048300	-1.193957	1.286719
31	8	0	4.793908	-1.464574	-0.619595
32	1	0	2.611511	1.221609	-0.026035
33	1	0	3.845450	-1.182293	1.840161

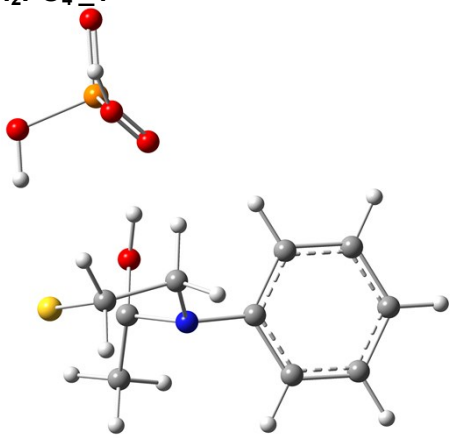
NBO analysis of **ts4·$H_2PO_4^-$** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
66. LP (1) O 25	/364. RY*(1) H 26	0.11	2.76	0.016
66. LP (1) O 25	/368. RY*(5) H 26	0.09	3.03	0.015
66. LP (1) O 25	/497. BD*(1) H 26 - O 27	12.47	1.24	0.111
67. LP (2) O 25	/497. BD*(1) H 26 - O 27	7.61	0.84	0.073
from unit 2 to unit 3				
70. LP (1) O 29	/ 78. LP*(1) H 32	16.99	0.76	0.115
70. LP (1) O 29	/458. RY*(1) H 32	1.17	2.18	0.046
70. LP (1) O 29	/459. RY*(2) H 32	0.19	2.34	0.019
70. LP (1) O 29	/460. RY*(3) H 32	0.14	2.30	0.016
70. LP (1) O 29	/461. RY*(4) H 32	0.32	2.66	0.026
71. LP (2) O 29	/459. RY*(2) H 32	0.13	2.08	0.015
71. LP (2) O 29	/460. RY*(3) H 32	0.73	2.04	0.035
72. LP (3) O 29	/ 78. LP*(1) H 32	371.39	0.72	0.478
72. LP (3) O 29	/458. RY*(1) H 32	14.13	2.15	0.171
72. LP (3) O 29	/459. RY*(2) H 32	0.62	2.31	0.037
72. LP (3) O 29	/461. RY*(4) H 32	0.14	2.62	0.019
72. LP (3) O 29	/462. RY*(5) H 32	0.23	2.82	0.025

int2·$H_2PO_4^-$_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.70820859 hartree/particle

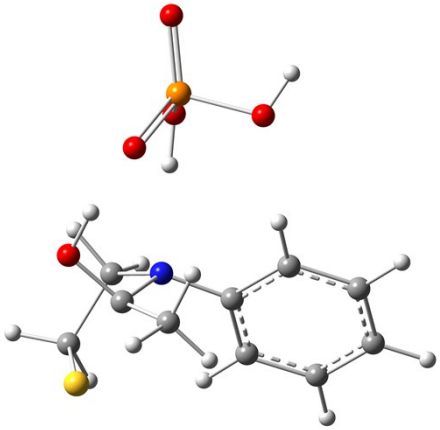
Thermal correction to Gibbs free energy: 0.205916 hartree/particle

Thermal correction to Enthalpy: 0.273503 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.620697	0.375484	0.178277
2	6	0	-4.660137	-0.527005	-0.066704
3	6	0	-4.377675	-1.882575	-0.258645
4	6	0	-3.050549	-2.322778	-0.211238
5	6	0	-2.007768	-1.422027	0.020470
6	6	0	-2.288359	-0.059450	0.222663
7	1	0	-3.827339	1.428839	0.348219
8	1	0	-5.688590	-0.172016	-0.097789
9	1	0	-5.183771	-2.589686	-0.444067
10	1	0	-2.819410	-3.373920	-0.370241
11	1	0	-0.976928	-1.767144	0.027021
12	7	0	-1.258802	0.906531	0.496986
13	6	0	-0.328167	0.527139	1.577258
14	1	0	-0.915707	0.322408	2.480438
15	1	0	0.272962	-0.356647	1.334681
16	6	0	0.584615	1.732591	1.784213
17	1	0	1.523432	1.437477	2.260108
18	1	0	0.094575	2.516037	2.371958
19	16	0	0.927427	2.358752	0.090548
20	6	0	-0.537497	1.417566	-0.696444
21	6	0	-1.398248	2.399310	-1.491613
22	1	0	-2.241409	1.861371	-1.940151
23	1	0	-1.772777	3.196963	-0.845358
24	1	0	-0.805141	2.834174	-2.302365
25	8	0	-0.092899	0.464796	-1.595654
26	1	0	0.494499	-0.227712	-1.160729
27	8	0	1.361027	-1.414475	-0.412412
28	15	0	2.830057	-1.419006	-0.007093
29	8	0	3.502192	-0.001355	-0.524531
30	8	0	2.797318	-1.204983	1.658746
31	8	0	3.782846	-2.533855	-0.316662
32	1	0	2.840875	0.718388	-0.480189
33	1	0	3.627717	-1.568119	2.004679

int2·$H_2PO_4^-$_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.70964343 hartree/particle

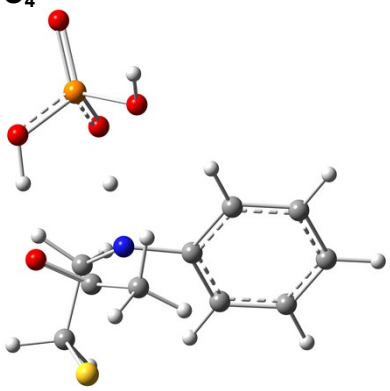
Thermal correction to Gibbs free energy: 0.207096 hartree/particle

Thermal correction to Enthalpy: 0.273505 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.846731	1.823402	0.348566
2	6	0	1.585073	2.987513	0.568892
3	6	0	2.939717	3.050780	0.226364
4	6	0	3.553354	1.928308	-0.334844
5	6	0	2.824238	0.753214	-0.539774
6	6	0	1.462347	0.686374	-0.202146
7	1	0	-0.213605	1.804081	0.585295
8	1	0	1.087199	3.856169	0.993886
9	1	0	3.507665	3.964279	0.389062
10	1	0	4.607096	1.957818	-0.605194
11	1	0	3.325078	-0.116180	-0.951238
12	6	0	0.969129	-1.286648	-1.618819
13	1	0	0.037203	-1.748682	-1.952198
14	1	0	1.330815	-0.626839	-2.411910
15	6	0	1.987761	-2.418328	-1.282129
16	1	0	3.006921	-2.168747	-1.597943
17	1	0	1.695446	-3.349053	-1.777464
18	16	0	1.953282	-2.619478	0.541216
19	6	0	0.463660	-1.439166	0.698317
20	6	0	0.459851	-0.809266	2.088559
21	1	0	1.367977	-0.237926	2.294279
22	1	0	-0.420885	-0.168057	2.192847
23	1	0	0.372853	-1.619368	2.819220
24	8	0	-0.668670	-2.203223	0.467373
25	1	0	-1.192844	0.198604	-1.065543
26	7	0	0.655967	-0.483142	-0.426569
27	8	0	-4.481019	0.825361	-0.532571
28	8	0	-2.687850	-0.563617	0.882921
29	15	0	-3.085354	0.574840	-0.045464
30	8	0	-2.555715	1.961180	0.748610
31	8	0	-2.072084	0.528881	-1.351636
32	1	0	-1.486729	-1.620954	0.617118
33	1	0	-3.089957	2.698044	0.412318

ts5·$H_2PO_4^-$



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.6893665 hartree/particle

Thermal correction to Gibbs free energy: 0.201561 hartree/particle

Thermal correction to Enthalpy: 0.267582 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.837861	1.950305	0.225174
2	6	0	1.638965	3.073963	0.433574
3	6	0	3.005855	3.037969	0.140565
4	6	0	3.563436	1.859570	-0.362047
5	6	0	2.768787	0.727776	-0.564006
6	6	0	1.396450	0.760713	-0.272378
7	1	0	-0.225669	1.992698	0.436882
8	1	0	1.185226	3.985325	0.816751
9	1	0	3.627092	3.917022	0.298319
10	1	0	4.626002	1.812011	-0.591800
11	1	0	3.226347	-0.183511	-0.929234
12	6	0	0.834407	-1.256269	-1.612859
13	1	0	-0.116731	-1.692309	-1.922063
14	1	0	1.216666	-0.646645	-2.436965
15	6	0	1.819741	-2.393589	-1.221474
16	1	0	2.815091	-2.229959	-1.650855
17	1	0	1.445774	-3.348423	-1.604180
18	16	0	1.962028	-2.440787	0.605340
19	6	0	0.266931	-1.389313	0.786612
20	6	0	0.337648	-0.648067	2.123827
21	1	0	1.272300	-0.099973	2.267773
22	1	0	-0.511845	0.039319	2.204680
23	1	0	0.240338	-1.403182	2.910774
24	8	0	-0.774147	-2.089216	0.550738
25	1	0	-0.690835	0.095875	-0.753006
26	7	0	0.516705	-0.366627	-0.468141
27	8	0	-4.306060	0.977141	-0.868951
28	8	0	-3.188308	-1.035962	0.272651
29	15	0	-3.030315	0.460989	-0.291132
30	8	0	-2.603874	1.362405	1.050573
31	8	0	-1.724949	0.533304	-1.142154
32	1	0	-2.291384	-1.475611	0.430997
33	1	0	-3.414826	1.621770	1.515664

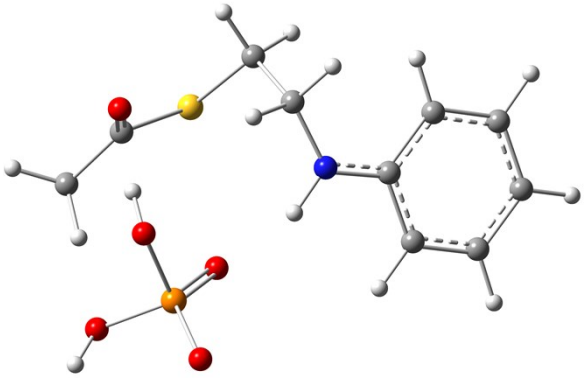
NBO analysis of **ts5·$H_2PO_4^-$** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
68. LP (1) N 26	/ 67. LP*(1) H 25	194.25	0.49	0.291
68. LP (1) N 26	/347. RY*(1) H 25	0.38	1.98	0.027
68. LP (1) N 26	/348. RY*(2) H 25	0.31	2.88	0.029
68. LP (1) N 26	/349. RY*(3) H 25	0.86	2.58	0.045
within unit 3				
72. LP (1) O 28	/458. RY*(1) H 32	1.99	2.63	0.065
73. LP (2) O 28	/460. RY*(3) H 32	1.06	2.05	0.042

3·$H_2PO_4^-$_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.71092327 hartree/particle

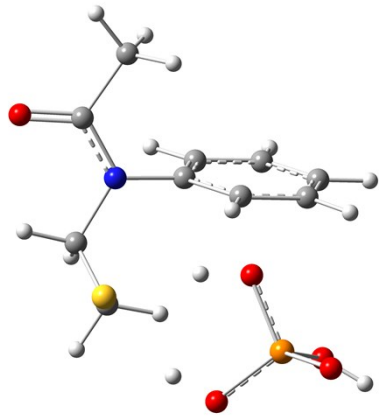
Thermal correction to Gibbs free energy: 0.199749 hartree/particle

Thermal correction to Enthalpy: 0.272959 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.813170	1.507703	0.620753
2	6	0	4.113348	1.852104	0.966898
3	6	0	5.213802	1.131975	0.473902
4	6	0	4.969296	0.052427	-0.378119
5	6	0	3.667969	-0.311155	-0.735093
6	6	0	2.552841	0.414117	-0.247380
7	1	0	1.969169	2.075181	1.005327
8	1	0	4.273542	2.698315	1.632980
9	1	0	6.228940	1.406429	0.750041
10	1	0	5.802701	-0.525863	-0.774846
11	1	0	3.519061	-1.157617	-1.399349
12	6	0	0.830866	-0.980937	-1.399502
13	1	0	-0.183069	-0.753218	-1.732267
14	1	0	1.455922	-1.069434	-2.303110
15	6	0	0.823953	-2.368429	-0.714492
16	1	0	1.841638	-2.710729	-0.499102
17	1	0	0.343986	-3.100961	-1.372803
18	16	0	-0.004346	-2.414775	0.921362
19	6	0	-1.710936	-2.111881	0.478122
20	6	0	-2.620645	-1.897449	1.663674
21	1	0	-2.171189	-2.243104	2.599700
22	1	0	-2.822545	-0.820746	1.738808
23	1	0	-3.569931	-2.413355	1.484569
24	8	0	-2.098219	-2.070559	-0.679405
25	1	0	0.487158	0.660196	-0.165520
26	7	0	1.259722	0.124000	-0.585059
27	8	0	-2.691156	3.141056	-0.496042
28	8	0	-3.068614	0.774966	-1.373078
29	15	0	-2.495882	1.701733	-0.120779
30	8	0	-3.587895	1.322970	1.103016
31	8	0	-1.189869	1.094177	0.353590
32	1	0	-2.837749	-0.161488	-1.227138
33	1	0	-4.336929	1.933361	1.016390

2·$H_2PO_4^-$_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.70723745 hartree/particle

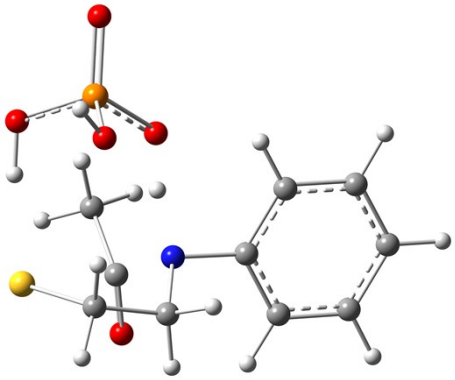
Thermal correction to Gibbs free energy: 0.195432 hartree/particle

Thermal correction to Enthalpy: 0.270808 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.651969	2.449558	1.249460
2	7	0	1.420173	1.638988	0.160832
3	16	0	-1.920372	1.474156	-0.503144
4	6	0	2.252439	1.783031	2.482890
5	6	0	0.785478	2.195118	-1.049754
6	6	0	-0.420661	1.404571	-1.576108
7	8	0	1.391186	3.653253	1.254109
8	1	0	-3.042150	-0.094203	-1.349495
9	6	0	1.988572	0.323204	0.065042
10	1	0	-0.133276	0.365156	-1.777624
11	1	0	1.551176	2.248918	-1.842998
12	1	0	0.485943	3.212152	-0.792802
13	1	0	-0.669524	1.849492	-2.548976
14	1	0	3.300263	1.507154	2.315463
15	1	0	2.201528	2.501824	3.303089
16	1	0	1.713387	0.870461	2.756492
17	6	0	3.325518	0.176958	-0.334280
18	6	0	1.216984	-0.814466	0.325069
19	6	0	1.781728	-2.086455	0.193224
20	6	0	3.890392	-1.094759	-0.456573
21	6	0	3.117207	-2.230722	-0.192676
22	1	0	1.161960	-2.959067	0.379943
23	1	0	3.914451	1.066690	-0.546012
24	1	0	4.929349	-1.198016	-0.762822
25	1	0	3.552460	-3.222389	-0.295447
26	8	0	-1.741492	-2.886807	-1.208008
27	15	0	-2.978243	-2.101670	-0.444510
28	8	0	-4.002984	-3.095149	-0.018693
29	8	0	-2.223071	-1.288831	0.699129
30	8	0	-3.491455	-1.002693	-1.486693
31	1	0	-2.053925	-3.777194	-1.433647
32	1	0	0.178646	-0.705779	0.618486
33	1	0	-2.031000	-0.305165	0.424092

ts6·$H_2PO_4^-$



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.68219737 hartree/particle

Thermal correction to Gibbs free energy: 0.199934 hartree/particle

Thermal correction to Enthalpy: 0.267555 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.725011	1.583656	0.878960
2	7	0	0.717121	0.473311	-0.218937
3	16	0	-1.366297	2.442090	-0.017505
4	6	0	0.267554	1.059949	2.228956
5	6	0	0.528791	1.129481	-1.546622
6	6	0	-0.889010	1.704659	-1.634821
7	8	0	1.575863	2.467599	0.782918
8	1	0	-2.642178	0.874556	0.557258
9	6	0	1.966275	-0.291045	-0.170901
10	1	0	-1.598450	0.921275	-1.916932
11	1	0	0.700714	0.373254	-2.321411
12	1	0	1.275559	1.924566	-1.655019
13	1	0	-0.908437	2.472093	-2.417991
14	1	0	1.109839	0.522951	2.690926
15	1	0	0.021996	1.914845	2.864138
16	1	0	-0.590082	0.390115	2.164175
17	6	0	3.209527	0.319975	-0.402105
18	6	0	1.918109	-1.663292	0.110886
19	6	0	3.098600	-2.412323	0.157277
20	6	0	4.383023	-0.435536	-0.353124
21	6	0	4.334733	-1.805429	-0.075478
22	1	0	3.043727	-3.476486	0.376192
23	1	0	3.251777	1.386385	-0.587726
24	1	0	5.339686	0.052543	-0.528220
25	1	0	5.250928	-2.391268	-0.039566
26	8	0	-2.978298	-1.103160	-1.495720
27	15	0	-2.640121	-1.299178	0.117006
28	8	0	-3.324706	-2.507485	0.659416
29	8	0	-1.074404	-1.288477	0.126052
30	8	0	-3.170040	0.047190	0.815739
31	1	0	-3.896950	-1.375005	-1.651055
32	1	0	0.958674	-2.138362	0.285216
33	1	0	-0.357080	-0.416325	-0.027836

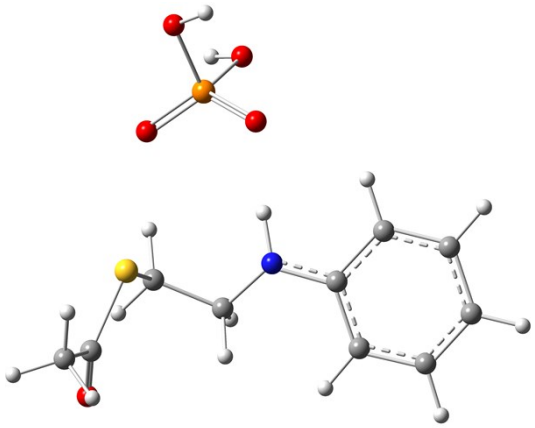
NBO analysis of **ts6·$H_2PO_4^-$** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 4				
61. LP (1) N 2	/ 79. LP*(1) H 33	144.35	0.51	0.258
61. LP (1) N 2	/465. RY*(2) H 33	0.65	3.02	0.042
61. LP (1) N 2	/466. RY*(3) H 33	0.65	2.61	0.039
from unit 3 to unit 2				
76. LP (1) O 30	/ 67. LP*(1) H 8	16.74	0.80	0.117
76. LP (1) O 30	/203. RY*(1) H 8	1.25	2.23	0.047
76. LP (1) O 30	/205. RY*(3) H 8	0.20	2.33	0.019
76. LP (1) O 30	/206. RY*(4) H 8	0.43	2.68	0.030
77. LP (2) O 30	/204. RY*(2) H 8	0.35	1.96	0.024
77. LP (2) O 30	/205. RY*(3) H 8	0.71	2.05	0.035
77. LP (2) O 30	/206. RY*(4) H 8	0.07	2.40	0.012
78. LP (3) O 30	/ 67. LP*(1) H 8	426.87	0.73	0.512
78. LP (3) O 30	/203. RY*(1) H 8	16.54	2.16	0.188
78. LP (3) O 30	/204. RY*(2) H 8	0.84	2.18	0.042
78. LP (3) O 30	/205. RY*(3) H 8	0.06	2.26	0.011
78. LP (3) O 30	/206. RY*(4) H 8	0.09	2.62	0.016
78. LP (3) O 30	/207. RY*(5) H 8	0.18	2.87	0.023

3·$H_2PO_4^-$_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1560.70386264 hartree/particle

Thermal correction to Gibbs free energy: 0.193763 hartree/particle

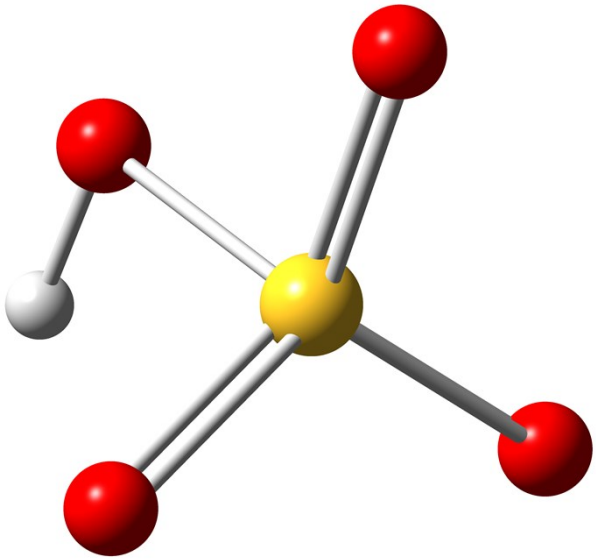
Thermal correction to Enthalpy: 0.272677 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.830451	-2.544412	0.318035
2	6	0	-2.893245	-3.438433	0.332752
3	6	0	-4.114977	-3.128666	-0.287881
4	6	0	-4.235000	-1.897474	-0.935309
5	6	0	-3.175256	-0.985302	-0.964611
6	6	0	-1.949484	-1.282485	-0.322398
7	1	0	-0.881762	-2.795249	0.785747
8	1	0	-2.766876	-4.398040	0.831772
9	1	0	-4.942433	-3.834260	-0.273387
10	1	0	-5.165975	-1.635553	-1.436525
11	1	0	-3.303575	-0.044214	-1.490106
12	6	0	-0.816137	0.783257	-1.086274
13	1	0	-0.697010	0.539252	-2.160352
14	1	0	-1.747758	1.354352	-0.994207
15	6	0	0.360165	1.678931	-0.695561
16	1	0	0.429876	2.517775	-1.393727
17	1	0	1.312616	1.133542	-0.698999
18	16	0	0.203288	2.409110	0.982593
19	6	0	-0.692789	3.905738	0.639362
20	6	0	-0.992600	4.733402	1.881398
21	1	0	-2.079843	4.781370	2.014446
22	1	0	-0.538706	4.319338	2.786217
23	1	0	-0.627967	5.754152	1.720605
24	8	0	-1.052029	4.266262	-0.470786
25	1	0	0.011830	-0.827116	0.011318
26	7	0	-0.887295	-0.410142	-0.271944
27	1	0	3.556364	-1.863963	1.984140
28	8	0	3.972784	-1.347450	1.275992
29	15	0	2.907952	-1.320402	-0.003588
30	8	0	3.438839	-2.604678	-0.921604
31	8	0	1.550417	-1.697884	0.553087
32	8	0	3.151662	-0.059571	-0.792645
33	1	0	4.043357	-2.245607	-1.590199

with HSO_4^-

HSO_4^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -699.78649264 hartree/particle

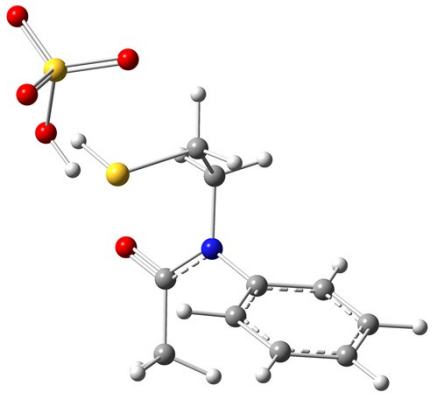
Thermal correction to Gibbs free energy: -0.002572 hartree/particle

Thermal correction to Enthalpy: 0.031963 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.155065	-0.024712	0.000020
2	8	0	-1.484034	0.475161	-0.000234
3	1	0	-1.993366	-0.353697	-0.000181
4	8	0	0.282453	-0.827961	1.244512
5	8	0	0.282964	-0.827672	-1.244602
6	8	0	0.857659	1.274108	0.000306

2·HSO_4^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.79522463 hartree/particle

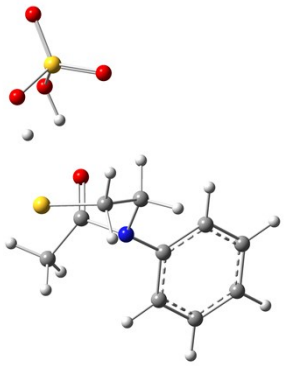
Thermal correction to Gibbs free energy: 0.188643 hartree/particle

Thermal correction to Enthalpy: 0.260082 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.229512	0.971635	0.177046
2	6	0	-4.591625	1.004595	0.488626
3	6	0	-5.322809	-0.183017	0.586961
4	6	0	-4.684170	-1.408778	0.372076
5	6	0	-3.325045	-1.444266	0.051514
6	6	0	-2.592519	-0.253857	-0.056693
7	1	0	-2.641857	1.883628	0.128407
8	1	0	-5.077863	1.960725	0.667755
9	1	0	-6.381217	-0.154794	0.835263
10	1	0	-5.244489	-2.337766	0.449274
11	1	0	-2.822807	-2.391965	-0.125229
12	7	0	-1.194003	-0.308046	-0.362979
13	6	0	-0.280664	-0.704317	0.725296
14	1	0	-0.578679	-1.702629	1.078903
15	1	0	0.725626	-0.788559	0.316725
16	6	0	-0.270439	0.248943	1.927107
17	1	0	0.486134	-0.122235	2.624692
18	1	0	-1.238002	0.246259	2.442305
19	16	0	0.086136	2.014082	1.549927
20	6	0	-0.689722	0.056839	-1.589463
21	6	0	-1.684149	0.489573	-2.659616
22	1	0	-2.599564	-0.109659	-2.665879
23	1	0	-1.971054	1.536073	-2.503061
24	1	0	-1.179974	0.412041	-3.624934
25	8	0	0.513434	0.032368	-1.849356
26	1	0	2.423580	0.078413	-1.426851
27	8	0	3.395451	0.056962	-1.293627
28	8	0	3.170280	1.584451	0.695731
29	8	0	2.885351	-0.860911	0.988602
30	8	0	5.148365	0.076861	0.430557
31	1	0	1.397921	1.840925	1.168051
32	16	0	3.685328	0.220465	0.344024

ts4·HSO_4^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.74194673 hartree/particle

Thermal correction to Gibbs free energy: 0.191865 hartree/particle

Thermal correction to Enthalpy: 0.258159 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.695078	0.590090	-0.361972
2	6	0	-4.920956	-0.053964	-0.530836
3	6	0	-5.096141	-1.375146	-0.104281
4	6	0	-4.019434	-2.042884	0.485535
5	6	0	-2.783158	-1.409932	0.636797
6	6	0	-2.598780	-0.076594	0.220717
7	1	0	-3.581544	1.628895	-0.654560
8	1	0	-5.750948	0.488335	-0.979855
9	1	0	-6.055668	-1.872524	-0.225868
10	1	0	-4.132874	-3.073538	0.816352
11	1	0	-1.948940	-1.955935	1.064810
12	7	0	-1.364127	0.608306	0.391940
13	6	0	-0.506699	0.185161	1.511131
14	1	0	-1.157145	-0.126927	2.337124
15	1	0	0.142035	-0.657596	1.239574
16	6	0	0.344216	1.387093	1.938715
17	1	0	1.133218	1.049318	2.620540
18	1	0	-0.286014	2.110789	2.469520
19	16	0	1.075706	2.210064	0.469913
20	6	0	-0.593918	0.772284	-0.854446
21	6	0	-1.075503	1.845833	-1.811223
22	1	0	-1.879504	1.427998	-2.435454
23	1	0	-1.437400	2.729854	-1.283848
24	1	0	-0.249724	2.122623	-2.470501
25	8	0	0.059573	-0.193360	-1.289148
26	1	0	1.624488	-0.732388	-1.359402
27	8	0	2.573076	-1.040791	-1.481482
28	8	0	3.602778	0.648969	0.078537
29	8	0	2.595287	-1.450350	0.990213
30	8	0	4.717186	-1.490903	-0.384801
31	1	0	2.684927	1.161140	0.242275
32	16	0	3.407637	-0.914961	-0.108142

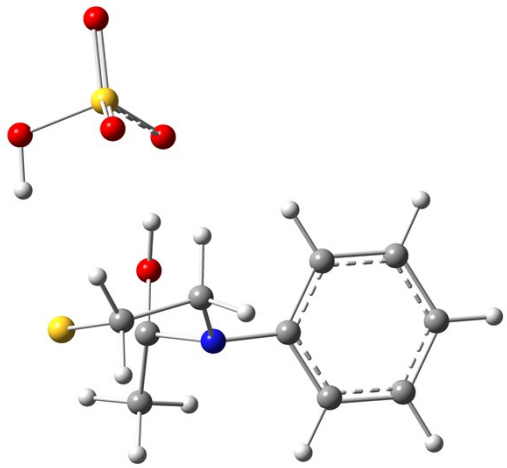
NBO analysis of **ts4·HSO_4^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
65. LP (1) O 25	/364. RY*(1) H 26	0.16	2.70	0.019
65. LP (1) O 25	/368. RY*(5) H 26	0.18	2.88	0.021
65. LP (1) O 25	/492. BD*(1) H 26 - O 27	18.89	1.21	0.135
66. LP (2) O 25	/365. RY*(2) H 26	0.07	2.05	0.011
from unit 2 to unit 3				
69. LP (1) O 28	/ 78. LP*(1) H 31	19.68	0.80	0.128
69. LP (1) O 28	/437. RY*(1) H 31	1.63	2.12	0.053
69. LP (1) O 28	/438. RY*(2) H 31	0.19	2.47	0.020
69. LP (1) O 28	/441. RY*(5) H 31	0.35	2.90	0.029
70. LP (2) O 28	/ 78. LP*(1) H 31	0.32	0.47	0.012
70. LP (2) O 28	/438. RY*(2) H 31	0.08	2.14	0.012
70. LP (2) O 28	/439. RY*(3) H 31	0.79	2.02	0.036
71. LP (3) O 28	/ 78. LP*(1) H 31	336.46	0.70	0.455
71. LP (3) O 28	/437. RY*(1) H 31	11.21	2.02	0.147
71. LP (3) O 28	/438. RY*(2) H 31	0.65	2.37	0.038
71. LP (3) O 28	/439. RY*(3) H 31	0.07	2.25	0.012
71. LP (3) O 28	/440. RY*(4) H 31	0.25	2.71	0.026
71. LP (3) O 28	/441. RY*(5) H 31	0.10	2.80	0.016

int2·HSO_4^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.78394230 hartree/particle

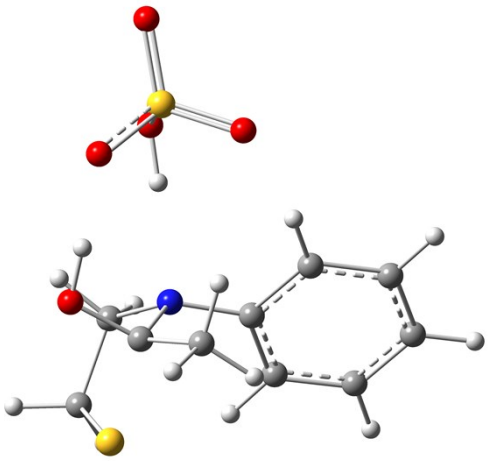
Thermal correction to Gibbs free energy: 0.196300 hartree/particle

Thermal correction to Enthalpy: 0.262569 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.584454	0.234928	0.312767
2	6	0	-4.597947	-0.706040	0.108604
3	6	0	-4.274147	-2.051846	-0.086628
4	6	0	-2.931385	-2.443870	-0.083176
5	6	0	-1.915679	-1.503602	0.106839
6	6	0	-2.236055	-0.150449	0.311291
7	1	0	-3.823820	1.280367	0.487507
8	1	0	-5.638931	-0.388544	0.113138
9	1	0	-5.060145	-2.788486	-0.239624
10	1	0	-2.667902	-3.487063	-0.243565
11	1	0	-0.875017	-1.814379	0.082241
12	7	0	-1.232794	0.852185	0.541785
13	6	0	-0.229615	0.507009	1.568020
14	1	0	-0.758394	0.269146	2.498566
15	1	0	0.400766	-0.345613	1.292487
16	6	0	0.643783	1.745897	1.738956
17	1	0	1.622587	1.476123	2.142169
18	1	0	0.161324	2.502110	2.366703
19	16	0	0.852408	2.409620	0.036465
20	6	0	-0.599858	1.409019	-0.676298
21	6	0	-1.545248	2.344687	-1.428890
22	1	0	-2.377806	1.764999	-1.843395
23	1	0	-1.931935	3.119291	-0.762289
24	1	0	-1.011684	2.813379	-2.261716
25	8	0	-0.155732	0.476908	-1.609482
26	1	0	0.501428	-0.160313	-1.218602
27	8	0	1.559194	-1.365400	-0.558290
28	8	0	3.464633	0.236772	-0.878699
29	8	0	2.947043	-0.722819	1.391005
30	8	0	3.934617	-2.140073	-0.431789
31	1	0	2.821149	0.951601	-0.678959
32	16	0	2.953437	-1.119334	-0.040093

int2·HSO_4^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.78534265 hartree/particle

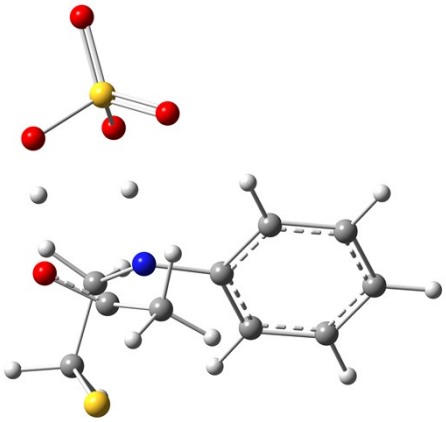
Thermal correction to Gibbs free energy: 0.197468 hartree/particle

Thermal correction to Enthalpy: 0.262504 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.658928	1.914565	0.277177
2	6	0	1.317026	3.127354	0.491782
3	6	0	2.673925	3.269392	0.184703
4	6	0	3.372735	2.177430	-0.335389
5	6	0	2.724661	0.955255	-0.536677
6	6	0	1.360783	0.810204	-0.233849
7	1	0	-0.403298	1.824849	0.495131
8	1	0	0.752920	3.970112	0.884618
9	1	0	3.178810	4.219973	0.343165
10	1	0	4.429808	2.267986	-0.577642
11	1	0	3.292320	0.114613	-0.919313
12	6	0	1.069298	-1.228872	-1.611289
13	1	0	0.192484	-1.763497	-1.982148
14	1	0	1.431154	-0.566689	-2.401889
15	6	0	2.143559	-2.278227	-1.182339
16	1	0	3.155434	-1.986078	-1.483517
17	1	0	1.921134	-3.251010	-1.630445
18	16	0	2.070193	-2.381639	0.649367
19	6	0	0.471550	-1.356926	0.679066
20	6	0	0.293711	-0.692907	2.040259
21	1	0	1.141707	-0.057584	2.306456
22	1	0	-0.624587	-0.096151	2.042666
23	1	0	0.191059	-1.486057	2.787065
24	8	0	-0.552908	-2.255189	0.392840
25	1	0	-1.203352	0.162246	-1.134106
26	7	0	0.634511	-0.416162	-0.462385
27	8	0	-4.425965	0.691197	-0.640028
28	8	0	-2.961968	-1.032663	0.429482
29	8	0	-2.511013	1.370630	0.834921
30	8	0	-2.109953	0.397333	-1.446270
31	1	0	-1.439812	-1.791082	0.440410
32	16	0	-3.100189	0.368979	-0.095741

ts5·HSO_4^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.75951280 hartree/particle

Thermal correction to Gibbs free energy: 0.192880 hartree/particle

Thermal correction to Enthalpy: 0.255853 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.878054	1.919560	0.270298
2	6	0	1.714436	3.016766	0.481926
3	6	0	3.072675	2.950665	0.155807
4	6	0	3.587545	1.768271	-0.381499
5	6	0	2.758020	0.662201	-0.586220
6	6	0	1.393986	0.726586	-0.263262
7	1	0	-0.178005	1.982225	0.517759
8	1	0	1.294341	3.930914	0.895331
9	1	0	3.720709	3.809638	0.316210
10	1	0	4.643086	1.697158	-0.636180
11	1	0	3.182898	-0.252920	-0.981222
12	6	0	0.778389	-1.268720	-1.612986
13	1	0	-0.181754	-1.674035	-1.935938
14	1	0	1.192754	-0.670809	-2.429899
15	6	0	1.716448	-2.440417	-1.209565
16	1	0	2.728025	-2.308406	-1.610605
17	1	0	1.320278	-3.380477	-1.605988
18	16	0	1.804930	-2.494023	0.619716
19	6	0	0.188057	-1.367478	0.766486
20	6	0	0.258628	-0.643565	2.113200
21	1	0	1.211098	-0.134304	2.281689
22	1	0	-0.565121	0.074395	2.186440
23	1	0	0.118122	-1.403809	2.888564
24	8	0	-0.893294	-2.032612	0.518924
25	1	0	-0.762750	0.136372	-0.804689
26	7	0	0.478488	-0.371844	-0.468215
27	8	0	-4.147974	1.070198	-0.811651
28	8	0	-3.157606	-0.896814	0.295610
29	8	0	-2.417413	1.392740	0.987823
30	8	0	-1.769780	0.505553	-1.234875
31	1	0	-2.229819	-1.367727	0.454686
32	16	0	-2.919441	0.613333	-0.164116

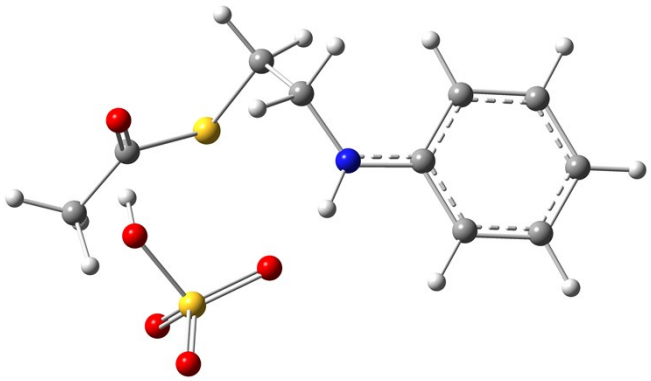
NBO analysis of **ts5·HSO_4^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
66. LP (1) N 26	/ 65. LP*(1) H 25	166.04	0.47	0.264
66. LP (1) N 26	/349. RY*(2) H 25	0.53	2.70	0.036
66. LP (1) N 26	/350. RY*(3) H 25	0.88	2.47	0.045
from unit 3 to unit 4				
70. LP (1) O 28	/ 79. LP*(1) H 31	19.92	0.89	0.134
70. LP (1) O 28	/438. RY*(1) H 31	2.15	2.78	0.069
70. LP (1) O 28	/439. RY*(2) H 31	0.42	2.84	0.031
70. LP (1) O 28	/440. RY*(3) H 31	0.31	2.54	0.025
70. LP (1) O 28	/441. RY*(4) H 31	0.17	2.73	0.020
71. LP (2) O 28	/439. RY*(2) H 31	0.06	2.49	0.012
71. LP (2) O 28	/440. RY*(3) H 31	0.57	2.19	0.032
71. LP (2) O 28	/441. RY*(4) H 31	0.18	2.38	0.019
72. LP (3) O 28	/ 79. LP*(1) H 31	376.45	0.75	0.488
72. LP (3) O 28	/438. RY*(1) H 31	5.15	2.64	0.115
72. LP (3) O 28	/439. RY*(2) H 31	0.51	2.70	0.037
72. LP (3) O 28	/440. RY*(3) H 31	0.19	2.40	0.021
72. LP (3) O 28	/441. RY*(4) H 31	0.12	2.59	0.017

3·HSO_4^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.78615938 hartree/particle

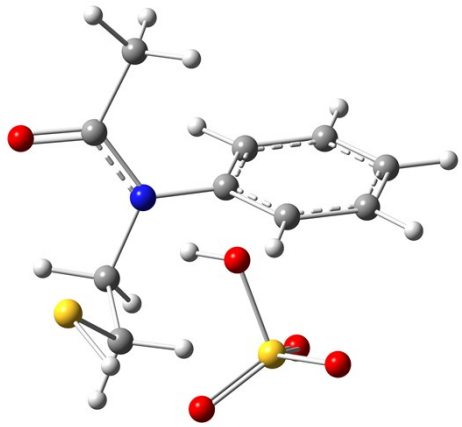
Thermal correction to Gibbs free energy: 0.189614 hartree/particle

Thermal correction to Enthalpy: 0.261876 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.692228	2.836926	-0.394979
2	6	0	2.669962	3.818145	-0.498705
3	6	0	3.950512	3.519369	-0.990872
4	6	0	4.221444	2.205088	-1.377439
5	6	0	3.250992	1.204162	-1.276678
6	6	0	1.957890	1.497792	-0.781825
7	1	0	0.701960	3.082187	-0.018625
8	1	0	2.429396	4.835106	-0.193882
9	1	0	4.711586	4.291752	-1.068806
10	1	0	5.205427	1.944485	-1.764490
11	1	0	3.500522	0.193334	-1.585277
12	6	0	1.033518	-0.793496	-1.153278
13	1	0	0.005062	-1.129751	-1.294033
14	1	0	1.524766	-0.832289	-2.141063
15	6	0	1.769373	-1.807205	-0.249747
16	1	0	2.839208	-1.582157	-0.188742
17	1	0	1.652557	-2.814260	-0.664860
18	16	0	1.236162	-1.842364	1.505457
19	6	0	-0.403942	-2.545613	1.378096
20	6	0	-1.151013	-2.601991	2.686323
21	1	0	-0.484736	-2.536607	3.551915
22	1	0	-1.838711	-1.743100	2.685075
23	1	0	-1.738885	-3.524828	2.725040
24	8	0	-0.885938	-2.904083	0.313759
25	1	0	0.021700	0.867946	-0.422012
26	7	0	0.967636	0.557446	-0.659857
27	8	0	-4.297600	1.028693	0.074244
28	8	0	-3.310184	-1.161481	-0.462060
29	8	0	-2.716494	-0.037807	1.707713
30	8	0	-1.854721	0.897144	-0.423804
31	1	0	-2.568232	-1.757467	-0.234376
32	16	0	-3.030248	0.315600	0.294864

2·HSO_4^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.78650456 hartree/particle

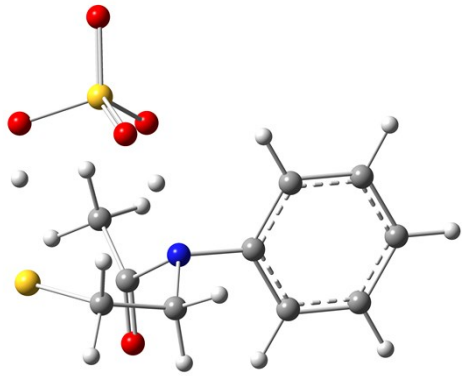
Thermal correction to Gibbs free energy: 0.187231 hartree/particle

Thermal correction to Enthalpy: 0.260197 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.299137	2.245785	1.079957
2	7	0	1.302552	1.411761	-0.019674
3	16	0	-2.009799	1.689610	-0.459571
4	6	0	1.869975	1.687326	2.376985
5	6	0	0.683600	1.876009	-1.273150
6	6	0	-0.656400	1.221287	-1.629316
7	8	0	0.847705	3.390445	1.036736
8	1	0	-2.853446	0.687077	-0.839878
9	6	0	2.093488	0.210612	-0.065364
10	1	0	-0.590331	0.130636	-1.647470
11	1	0	1.389339	1.672921	-2.089325
12	1	0	0.566764	2.959001	-1.181256
13	1	0	-0.928802	1.561858	-2.635184
14	1	0	2.958749	1.813895	2.406329
15	1	0	1.435325	2.262249	3.197553
16	1	0	1.653668	0.623908	2.510756
17	6	0	3.492586	0.317235	-0.110752
18	6	0	1.490974	-1.051860	-0.109702
19	6	0	2.291783	-2.196457	-0.188588
20	6	0	4.286193	-0.829795	-0.174025
21	6	0	3.684757	-2.092746	-0.213585
22	1	0	1.805970	-3.167621	-0.228956
23	1	0	3.950470	1.303820	-0.097076
24	1	0	5.369812	-0.736272	-0.201395
25	1	0	4.299766	-2.988314	-0.268817
26	8	0	-1.364575	-2.104724	-0.880725
27	8	0	-3.274405	-3.445771	0.034878
28	8	0	-2.491153	-1.458036	1.271906
29	8	0	-3.657508	-1.162515	-0.939437
30	1	0	0.410684	-1.168708	-0.099375
31	1	0	-2.208591	-0.531555	1.131427
32	16	0	-2.724639	-2.115766	-0.267102

ts6·HSO_4^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.74672157 hartree/particle

Thermal correction to Gibbs free energy: 0.190549 hartree/particle

Thermal correction to Enthalpy: 0.256044 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.696040	1.643938	0.859228
2	7	0	0.672446	0.508699	-0.178777
3	16	0	-1.584912	2.350184	-0.078318
4	6	0	0.278675	1.204866	2.247534
5	6	0	0.453283	1.099216	-1.537190
6	6	0	-0.975664	1.650446	-1.670243
7	8	0	1.446663	2.593394	0.669434
8	1	0	-2.749200	0.795453	0.335341
9	6	0	1.936217	-0.240397	-0.138160
10	1	0	-1.648549	0.855683	-2.001140
11	1	0	0.635185	0.305899	-2.270545
12	1	0	1.193212	1.893454	-1.687446
13	1	0	-0.970426	2.430746	-2.440633
14	1	0	1.146173	0.728255	2.730234
15	1	0	0.015976	2.094773	2.824124
16	1	0	-0.553472	0.501590	2.240100
17	6	0	3.174468	0.397714	-0.315590
18	6	0	1.901694	-1.626683	0.063947
19	6	0	3.090316	-2.363413	0.085227
20	6	0	4.356860	-0.345106	-0.288307
21	6	0	4.321897	-1.729066	-0.090627
22	1	0	3.045493	-3.438781	0.242189
23	1	0	3.204131	1.472590	-0.450300
24	1	0	5.309459	0.163439	-0.421612
25	1	0	5.244757	-2.304905	-0.072731
26	8	0	-2.502926	-1.328861	-1.468071
27	8	0	-3.157591	-2.522792	0.650434
28	8	0	-1.065944	-1.218183	0.561184
29	8	0	-3.291934	-0.071128	0.559743
30	1	0	0.947987	-2.123335	0.205086
31	1	0	-0.399229	-0.402219	0.149860
32	16	0	-2.537431	-1.369063	0.002830

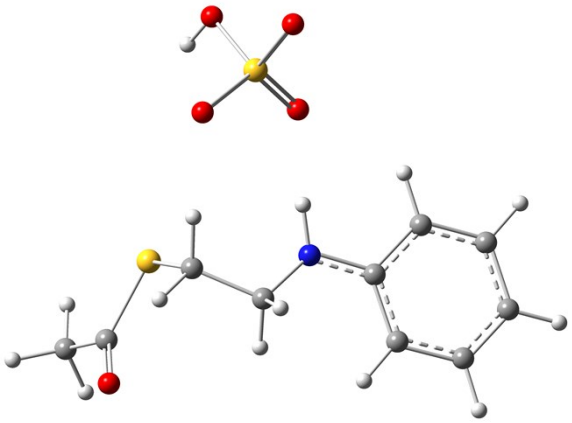
NBO analysis of **ts6·HSO_4^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 4				
60. LP (1) N 2	/ 79. LP*(1) H 31	132.75	0.49	0.243
60. LP (1) N 2	/438. RY*(1) H 31	0.06	1.88	0.010
60. LP (1) N 2	/439. RY*(2) H 31	0.70	2.96	0.043
60. LP (1) N 2	/440. RY*(3) H 31	0.74	2.51	0.041
from unit 3 to unit 2				
76. LP (1) O 29	/ 66. LP*(1) H 8	19.57	0.82	0.129
76. LP (1) O 29	/203. RY*(1) H 8	1.68	2.14	0.054
76. LP (1) O 29	/205. RY*(3) H 8	0.14	2.41	0.017
76. LP (1) O 29	/206. RY*(4) H 8	0.22	3.41	0.025
76. LP (1) O 29	/207. RY*(5) H 8	0.21	2.35	0.020
77. LP (2) O 29	/204. RY*(2) H 8	0.31	2.04	0.023
77. LP (2) O 29	/205. RY*(3) H 8	0.61	2.07	0.032
77. LP (2) O 29	/207. RY*(5) H 8	0.06	2.01	0.010
78. LP (3) O 29	/ 66. LP*(1) H 8	366.48	0.71	0.474
78. LP (3) O 29	/203. RY*(1) H 8	12.85	2.04	0.159
78. LP (3) O 29	/204. RY*(2) H 8	0.97	2.27	0.046
78. LP (3) O 29	/205. RY*(3) H 8	0.12	2.30	0.017
78. LP (3) O 29	/207. RY*(5) H 8	0.31	2.24	0.026

3·HSO_4^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1616.77956168 hartree/particle

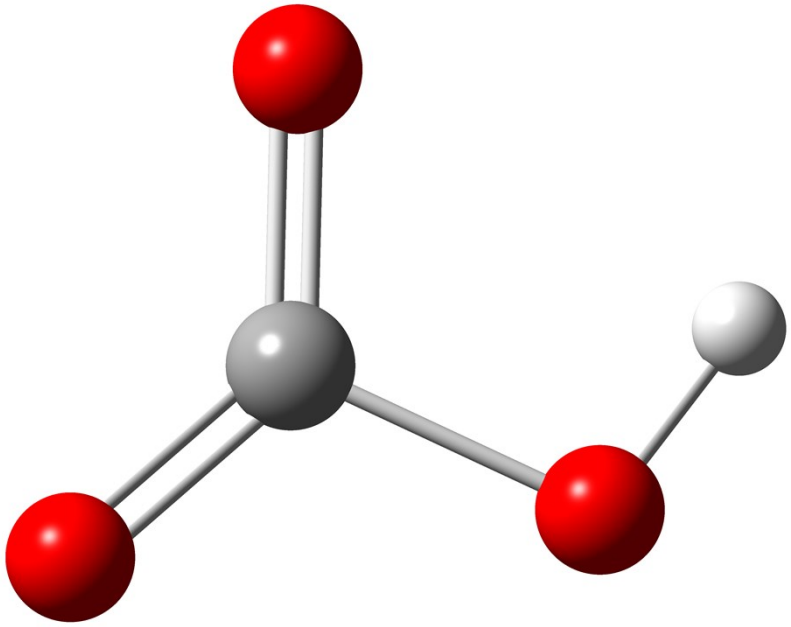
Thermal correction to Gibbs free energy: 0.184020 hartree/particle

Thermal correction to Enthalpy: 0.261726 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.113936	3.550625	1.418760
2	7	0	0.985463	-0.307053	-0.473027
3	16	0	-0.728856	1.889828	1.234813
4	6	0	-0.145202	4.055506	2.853613
5	6	0	0.817837	1.041799	-0.968524
6	6	0	-0.539312	1.624091	-0.573054
7	8	0	0.299323	4.242685	0.502828
8	1	0	-3.443170	-1.582953	1.067082
9	6	0	2.176828	-0.995142	-0.564239
10	1	0	-1.362975	0.960536	-0.861714
11	1	0	0.884678	1.085149	-2.073194
12	1	0	1.614977	1.685216	-0.577940
13	1	0	-0.678080	2.598892	-1.048577
14	1	0	-0.729812	4.981831	2.887206
15	1	0	-0.572354	3.328125	3.549622
16	1	0	0.879228	4.292944	3.162878
17	6	0	3.407732	-0.377862	-0.885305
18	6	0	2.184944	-2.388970	-0.300885
19	6	0	3.370802	-3.111970	-0.334567
20	6	0	4.591830	-1.121745	-0.910585
21	6	0	4.593632	-2.490144	-0.634325
22	1	0	3.341216	-4.180743	-0.129693
23	1	0	3.445545	0.681849	-1.117312
24	1	0	5.523826	-0.615610	-1.158100
25	1	0	5.517789	-3.062602	-0.660142
26	8	0	-2.922116	-0.521423	-1.318877
27	8	0	-3.101741	-2.961873	-1.888608
28	8	0	-1.309399	-2.124051	-0.343827
29	8	0	-3.713801	-2.212537	0.375593
30	1	0	1.240236	-2.879905	-0.080792
31	1	0	0.142808	-0.891300	-0.465722
32	16	0	-2.673512	-1.935604	-0.929051

HCO_3^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -264.55203985 hartree/particle

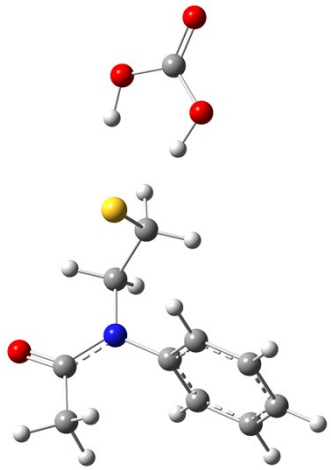
Thermal correction to Gibbs free energy: 0.000121 hartree/particle

Thermal correction to Enthalpy: 0.030397 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.157500	-0.067242	-0.000011
2	8	0	0.098932	-1.298861	0.000025
3	8	0	1.026027	0.768506	0.000069
4	1	0	1.746370	0.117346	-0.000485
5	8	0	-1.225130	0.566118	-0.000025

2·HCO_3^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.5544092 hartree/particle

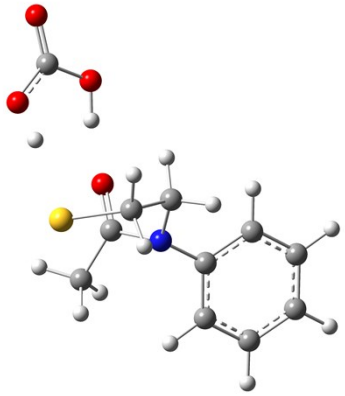
Thermal correction to Gibbs free energy: 0.190581 hartree/particle

Thermal correction to Enthalpy: 0.260117 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.417697	1.264752	-0.687662
2	6	0	-1.858163	2.586350	-0.800731
3	6	0	-2.953219	3.037509	-0.056775
4	6	0	-3.605325	2.161580	0.816702
5	6	0	-3.163202	0.841551	0.939683
6	6	0	-2.076905	0.384116	0.180166
7	1	0	-0.554793	0.900398	-1.242655
8	1	0	-1.337827	3.265874	-1.471793
9	1	0	-3.291995	4.066966	-0.151046
10	1	0	-4.452452	2.505688	1.406265
11	1	0	-3.657228	0.155163	1.623641
12	7	0	-1.636775	-0.975058	0.318062
13	6	0	-0.511087	-1.258585	1.232431
14	1	0	-0.848069	-1.067513	2.266187
15	1	0	-0.310049	-2.325776	1.131997
16	6	0	0.764544	-0.450007	0.965534
17	1	0	1.470574	-0.737178	1.756153
18	1	0	0.563283	0.619766	1.107673
19	16	0	1.527078	-0.741072	-0.690558
20	6	0	-2.339194	-2.020267	-0.235930
21	6	0	-3.424884	-1.666538	-1.247757
22	1	0	-4.333118	-1.316570	-0.742558
23	1	0	-3.109397	-0.881778	-1.941827
24	1	0	-3.663800	-2.577444	-1.800641
25	8	0	-2.118409	-3.198478	0.049784
26	1	0	3.551686	-1.002469	-0.076049
27	8	0	4.514371	-0.849178	0.196622
28	8	0	3.907033	1.255586	-0.448735
29	1	0	3.042382	0.748493	-0.598895
30	6	0	4.865494	0.440092	0.029798
31	8	0	5.981106	0.842773	0.295239

ts4·HCO_3^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.52317331 hartree/particle

Thermal correction to Gibbs free energy: 0.194169 hartree/particle

Thermal correction to Enthalpy: 0.258217 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.235337	-0.745335	-0.310183
2	6	0	4.547244	-0.288526	-0.441466
3	6	0	4.889531	1.016992	-0.073094
4	6	0	3.892004	1.862028	0.421565
5	6	0	2.573129	1.416849	0.535005
6	6	0	2.217962	0.100927	0.174311
7	1	0	2.992508	-1.773324	-0.555786
8	1	0	5.311905	-0.967576	-0.813853
9	1	0	5.914985	1.366834	-0.166356
10	1	0	4.134764	2.883963	0.706493
11	1	0	1.803783	2.095942	0.888914
12	7	0	0.887818	-0.370845	0.313266
13	6	0	0.070986	0.122197	1.429213
14	1	0	0.747706	0.472547	2.217334
15	1	0	-0.564315	0.965686	1.126856
16	6	0	-0.787742	-1.042513	1.953740
17	1	0	-1.527756	-0.643486	2.660254
18	1	0	-0.138253	-1.734165	2.505848
19	16	0	-1.613842	-1.959680	0.595266
20	6	0	0.127052	-0.572471	-0.909545
21	6	0	0.592176	-1.671341	-1.842757
22	1	0	1.414351	-1.294527	-2.469719
23	1	0	0.920292	-2.557959	-1.298423
24	1	0	-0.240378	-1.933377	-2.498776
25	8	0	-0.618768	0.322642	-1.332495
26	1	0	-2.071159	1.051260	-0.689430
27	8	0	-2.794668	1.678438	-0.434598
28	8	0	-4.071445	-0.213400	-0.171974
29	1	0	-3.195176	-0.689627	0.041615
30	6	0	-4.013454	1.117743	-0.275537
31	8	0	-5.010352	1.813484	-0.228382

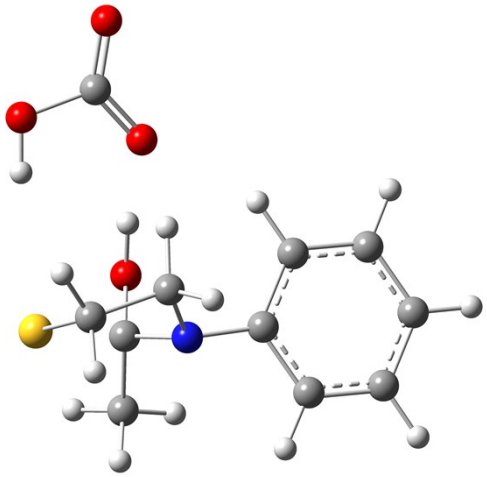
NBO analysis of **ts4·HCO_3^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
60. LP (1) O 25	/359. RY*(5) H 26	0.09	2.90	0.015
60. LP (1) O 25	/462. BD*(1) H 26 - O 27	10.09	1.25	0.100
61. LP (2) O 25	/462. BD*(1) H 26 - O 27	3.91	0.83	0.052
from unit 2 to unit 3				
64. LP (1) O 28	/ 67. LP*(1) H 29	14.99	0.76	0.108
64. LP (1) O 28	/394. RY*(1) H 29	1.30	2.11	0.047
64. LP (1) O 28	/396. RY*(3) H 29	0.20	2.46	0.020
64. LP (1) O 28	/398. RY*(5) H 29	0.20	3.13	0.023
65. LP (2) O 28	/ 67. LP*(1) H 29	3.04	0.50	0.038
65. LP (2) O 28	/395. RY*(2) H 29	0.91	2.00	0.040
65. LP (2) O 28	/396. RY*(3) H 29	0.14	2.21	0.016
66. LP (3) O 28	/ 67. LP*(1) H 29	420.50	0.70	0.498
66. LP (3) O 28	/394. RY*(1) H 29	17.87	2.05	0.190
66. LP (3) O 28	/395. RY*(2) H 29	0.21	2.20	0.021
66. LP (3) O 28	/396. RY*(3) H 29	0.99	2.40	0.048
66. LP (3) O 28	/397. RY*(4) H 29	0.32	2.37	0.027
66. LP (3) O 28	/398. RY*(5) H 29	0.20	3.08	0.024

int2·HCO_3^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.54627580 hartree/particle

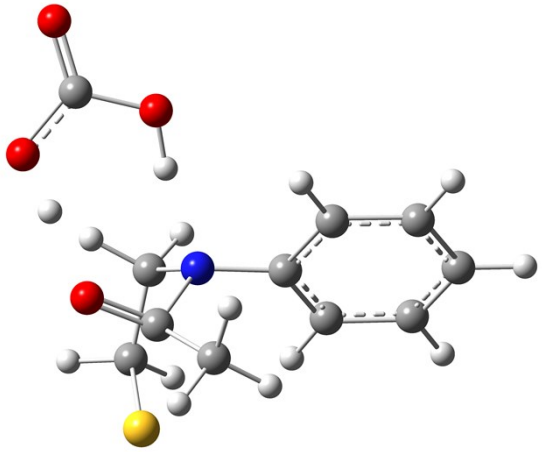
Thermal correction to Gibbs free energy: 0.196477 hartree/particle

Thermal correction to Enthalpy: 0.260507 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.084732	-0.479835	0.327663
2	6	0	4.179277	0.370954	0.146322
3	6	0	3.974486	1.741405	-0.039299
4	6	0	2.670503	2.248074	-0.048623
5	6	0	1.572424	1.399937	0.120219
6	6	0	1.775352	0.022387	0.313819
7	1	0	3.228995	-1.544517	0.491796
8	1	0	5.188853	-0.035668	0.159322
9	1	0	4.823164	2.408815	-0.175779
10	1	0	2.500258	3.311632	-0.201643
11	1	0	0.561525	1.799715	0.084415
12	7	0	0.688968	-0.897201	0.525771
13	6	0	-0.259469	-0.507880	1.584582
14	1	0	0.306046	-0.335732	2.508352
15	1	0	-0.824019	0.400398	1.334903
16	6	0	-1.209335	-1.692904	1.735094
17	1	0	-2.147111	-1.400475	2.216769
18	1	0	-0.745126	-2.510163	2.297644
19	16	0	-1.551191	-2.233066	0.013601
20	6	0	-0.015755	-1.346514	-0.704082
21	6	0	0.827364	-2.347678	-1.493264
22	1	0	1.715879	-1.840612	-1.886892
23	1	0	1.132139	-3.183968	-0.859207
24	1	0	0.248530	-2.724974	-2.342236
25	8	0	-0.389008	-0.354053	-1.589058
26	1	0	-0.944293	0.367842	-1.146324
27	8	0	-1.673220	1.628489	-0.423039
28	8	0	-3.748346	0.741662	-0.190828
29	1	0	-3.190474	-0.031731	-0.392584
30	6	0	-2.903168	1.870956	-0.163158
31	8	0	-3.443996	2.940839	0.120151

int2·HCO_3^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.53191259 hartree/particle

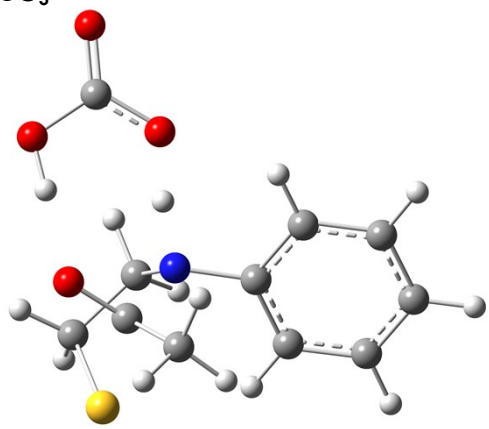
Thermal correction to Gibbs free energy: 0.195288 hartree/particle

Thermal correction to Enthalpy: 0.259450 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269213	-1.821068	0.455232
2	6	0	-2.431294	-2.590221	0.533268
3	6	0	-3.622922	-2.129495	-0.035656
4	6	0	-3.635292	-0.888045	-0.677055
5	6	0	-2.476686	-0.108716	-0.742425
6	6	0	-1.273667	-0.565436	-0.176940
7	1	0	-0.339052	-2.196011	0.871498
8	1	0	-2.399217	-3.559612	1.026126
9	1	0	-4.527687	-2.731321	0.016716
10	1	0	-4.556006	-0.511783	-1.118788
11	1	0	-2.516225	0.867856	-1.208835
12	6	0	0.244881	0.891764	-1.478877
13	1	0	1.331730	0.970474	-1.562651
14	1	0	-0.112575	0.289408	-2.320551
15	6	0	-0.357364	2.327895	-1.489354
16	1	0	-1.290958	2.361014	-2.065098
17	1	0	0.348251	3.009495	-1.977717
18	16	0	-0.665490	2.838639	0.240564
19	6	0	0.325929	1.060392	0.935164
20	6	0	-0.402310	0.747207	2.243860
21	1	0	-0.022862	-0.198341	2.654201
22	1	0	-0.148121	1.542971	2.949381
23	1	0	-1.488123	0.691130	2.137684
24	8	0	1.591731	1.255979	1.035191
25	1	0	1.398232	-1.008131	-0.123953
26	7	0	-0.041746	0.167666	-0.226867
27	8	0	3.548310	0.004891	-0.054662
28	8	0	2.074395	-1.740246	-0.180427
29	1	0	2.736007	0.497991	0.340663
30	6	0	3.354877	-1.295898	-0.259363
31	8	0	4.258693	-2.069037	-0.515945

ts5·HCO_3^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.52562302 hartree/particle

Thermal correction to Gibbs free energy: 0.193219 hartree/particle

Thermal correction to Enthalpy: 0.255691 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.202719	-1.934296	0.244961
2	6	0	-2.385424	-2.673021	0.342022
3	6	0	-3.613773	-2.097729	0.005877
4	6	0	-3.649485	-0.769534	-0.431436
5	6	0	-2.473091	-0.023905	-0.530929
6	6	0	-1.238988	-0.600665	-0.190040
7	1	0	-0.245011	-2.387702	0.481594
8	1	0	-2.339378	-3.707825	0.674471
9	1	0	-4.531931	-2.676684	0.080273
10	1	0	-4.598927	-0.305709	-0.691824
11	1	0	-2.507015	1.016803	-0.837365
12	6	0	0.245633	0.825392	-1.568119
13	1	0	1.117061	0.354196	-2.037790
14	1	0	-0.619522	0.650997	-2.212256
15	6	0	0.472103	2.337224	-1.382952
16	1	0	0.173658	2.880983	-2.284825
17	1	0	1.522647	2.551023	-1.168890
18	16	0	-0.539930	2.855129	0.043494
19	6	0	0.287796	1.237906	0.966450
20	6	0	-0.556247	0.919071	2.200005
21	1	0	-0.232198	-0.040666	2.620427
22	1	0	-0.345615	1.701279	2.935835
23	1	0	-1.630595	0.888116	2.003367
24	8	0	1.535742	1.360139	1.123362
25	1	0	0.952403	-0.666748	-0.111577
26	7	0	0.004561	0.143728	-0.251911
27	8	0	3.518783	-0.135237	0.037789
28	8	0	1.790311	-1.605299	-0.092362
29	1	0	2.788926	0.413445	0.431919
30	6	0	3.080610	-1.403059	-0.221649
31	8	0	3.895372	-2.257181	-0.557085

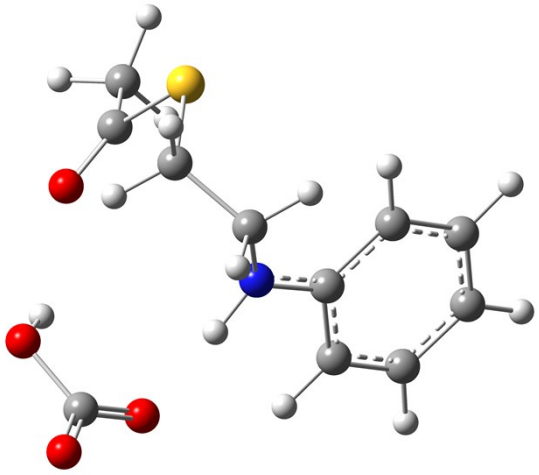
NBO analysis of **ts5·HCO_3^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
62. LP (1) N 26	/ 61. LP*(1) H 25	241.70	0.49	0.324
62. LP (1) N 26	/338. RY*(1) H 25	1.72	2.96	0.069
62. LP (1) N 26	/340. RY*(3) H 25	0.63	2.59	0.039
within unit 3				
63. LP (1) O 27	/394. RY*(1) H 29	1.90	2.61	0.063
64. LP (2) O 27	/395. RY*(2) H 29	1.10	1.98	0.043

3·HCO_3^-_1



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.54527444 hartree/particle

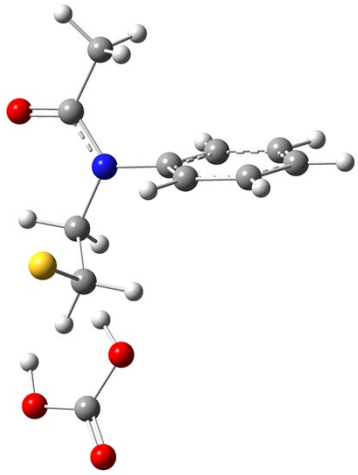
Thermal correction to Gibbs free energy: 0.187849 hartree/particle

Thermal correction to Enthalpy: 0.260002 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.405852	-2.350935	-0.072281
2	6	0	-2.601502	-3.005010	0.199749
3	6	0	-3.839523	-2.405443	-0.080733
4	6	0	-3.841375	-1.123959	-0.637904
5	6	0	-2.649709	-0.446854	-0.909607
6	6	0	-1.396678	-1.047440	-0.636850
7	1	0	-0.451275	-2.829340	0.133140
8	1	0	-2.567823	-4.004956	0.629485
9	1	0	-4.771821	-2.924068	0.129842
10	1	0	-4.786436	-0.629849	-0.860025
11	1	0	-2.696972	0.560786	-1.310914
12	6	0	0.051355	0.679789	-1.735549
13	1	0	0.776797	0.381927	-2.509394
14	1	0	-0.870521	0.961321	-2.255050
15	6	0	0.656102	1.905295	-1.027453
16	1	0	0.861529	2.701862	-1.752015
17	1	0	1.594721	1.640678	-0.531327
18	16	0	-0.450298	2.623971	0.248420
19	6	0	0.249762	1.966388	1.769031
20	6	0	-0.624274	2.223667	2.983316
21	1	0	-1.231718	1.327666	3.160641
22	1	0	0.014217	2.387768	3.856550
23	1	0	-1.298217	3.073727	2.839630
24	8	0	1.302409	1.368083	1.833413
25	1	0	0.663109	-1.013165	-0.677002
26	7	0	-0.183375	-0.439352	-0.855016
27	8	0	3.566224	-0.107786	-0.044309
28	8	0	2.200414	-1.847600	-0.535533
29	1	0	2.856973	-0.057315	0.619838
30	6	0	3.293256	-1.266181	-0.827905
31	8	0	4.144007	-1.532800	-1.683047

2·HCO_3^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.55454273 hartree/particle

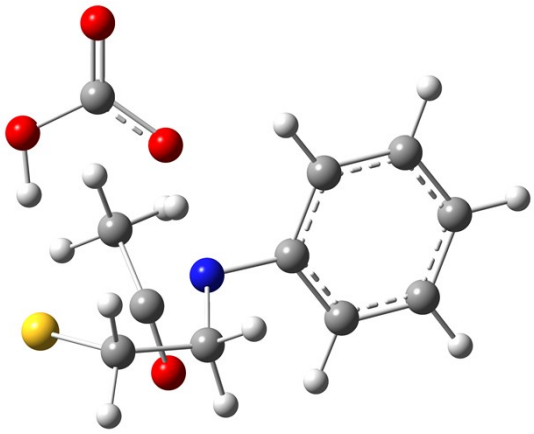
Thermal correction to Gibbs free energy: 0.189972 hartree/particle

Thermal correction to Enthalpy: 0.255505 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.770530	-1.312186	0.550596
2	7	0	-1.805276	-0.638358	-0.160331
3	16	0	1.341388	-1.544262	0.489407
4	6	0	-3.529503	-0.519433	1.610263
5	6	0	-0.984165	-1.369765	-1.147082
6	6	0	0.518812	-1.069972	-1.094479
7	8	0	-3.028949	-2.502705	0.362868
8	1	0	3.324356	-1.806834	-0.266190
9	6	0	-1.695731	0.792504	-0.113153
10	1	0	0.695203	-0.009265	-1.315785
11	1	0	-1.362314	-1.132241	-2.156757
12	1	0	-1.164954	-2.428549	-0.957670
13	1	0	0.963821	-1.634775	-1.924456
14	1	0	-2.872354	0.127508	2.198898
15	1	0	-4.293899	0.117700	1.149053
16	1	0	-4.024996	-1.239968	2.264334
17	6	0	-2.594843	1.582064	-0.843672
18	6	0	-0.682549	1.405599	0.634772
19	6	0	-0.584364	2.799526	0.659079
20	6	0	-2.497991	2.975849	-0.810083
21	6	0	-1.491720	3.587814	-0.055964
22	1	0	0.211530	3.267866	1.233202
23	1	0	-3.368191	1.095790	-1.434112
24	1	0	-3.202688	3.580930	-1.376585
25	1	0	-1.410075	4.672327	-0.033470
26	8	0	3.785665	0.374799	0.344839
27	8	0	4.280020	-1.659237	-0.565942
28	1	0	0.028595	0.772808	1.162409
29	1	0	2.912078	-0.121857	0.483583
30	6	0	4.688380	-0.409971	-0.273563
31	8	0	5.804014	-0.015207	-0.550242

ts6·HCO_3^-



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.52137321 hartree/particle

Thermal correction to Gibbs free energy: 0.192951 hartree/particle

Thermal correction to Enthalpy: 0.255505 hartree/particle

Number of imaginary frequencies: 1

IRC calc: OK

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.628156	1.674612	0.796276
2	7	0	0.716219	0.532010	-0.313512
3	16	0	-1.332907	2.407691	-0.062866
4	6	0	0.220946	1.078507	2.138696
5	6	0	0.575946	1.205187	-1.634510
6	6	0	-0.838841	1.789484	-1.723930
7	8	0	1.497555	2.555658	0.736642
8	1	0	-2.373274	0.530392	0.450053
9	6	0	1.968353	-0.213063	-0.203056
10	1	0	-1.542638	1.019893	-2.057146
11	1	0	0.754290	0.462481	-2.419971
12	1	0	1.329175	1.997108	-1.708084
13	1	0	-0.853015	2.605757	-2.454674
14	1	0	1.102801	0.596881	2.584112
15	1	0	-0.085756	1.895712	2.797827
16	1	0	-0.590091	0.351442	2.065534
17	6	0	3.214105	0.423194	-0.325837
18	6	0	1.919912	-1.593710	0.035525
19	6	0	3.105270	-2.326953	0.149666
20	6	0	4.392378	-0.318020	-0.209100
21	6	0	4.345442	-1.695485	0.027994
22	1	0	3.051558	-3.398097	0.331797
23	1	0	3.250704	1.495310	-0.476288
24	1	0	5.351689	0.187834	-0.298585
25	1	0	5.265878	-2.269087	0.116623
26	8	0	-1.056203	-1.241998	-0.358587
27	8	0	-2.854222	-0.306912	0.695283
28	1	0	0.954428	-2.083798	0.112879
29	1	0	-0.305520	-0.312510	-0.241076
30	6	0	-2.219630	-1.420433	0.230996
31	8	0	-2.756120	-2.511465	0.374778

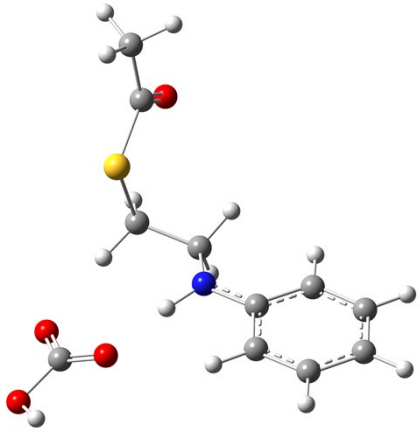
NBO analysis of **ts6·HCO_3^-** (excerpt)

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 3				
56. LP (1) N 2	/ 67. LP*(1) H 29	189.55	0.51	0.294
56. LP (1) N 2	/394. RY*(1) H 29	0.09	1.87	0.012
56. LP (1) N 2	/395. RY*(2) H 29	1.14	3.09	0.057
56. LP (1) N 2	/396. RY*(3) H 29	0.64	2.63	0.039
within unit 2				
65. LP (1) O 27	/193. RY*(1) H 8	1.48	2.14	0.051
66. LP (2) O 27	/194. RY*(2) H 8	1.02	2.02	0.042

3·HCO_3^-_2



Level of theory: M06-2X/6-311+G(d,p) in PCM (water)//B3LYP/6-31+G(d), 1 atm, 298.15 K

Energy: -1181.54527444 hartree/particle

Thermal correction to Gibbs free energy: 0.187982 hartree/particle

Thermal correction to Enthalpy: 0.260105 hartree/particle

Number of imaginary frequencies: 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.524438	-1.486787	0.157010
2	7	0	-0.711938	-0.174196	-0.234594
3	16	0	2.453716	-0.151049	0.634846
4	6	0	4.367746	-2.030447	1.302459
5	6	0	0.322706	-0.565848	-1.166028
6	6	0	1.606499	0.235759	-0.948648
7	8	0	3.604588	-1.950750	-0.970029
8	1	0	-1.291353	4.662873	0.972831
9	6	0	-1.904667	-0.845774	-0.122951
10	1	0	1.403042	1.315856	-0.922685
11	1	0	0.010146	-0.403053	-2.216518
12	1	0	0.538132	-1.636806	-1.064002
13	1	0	2.322207	0.016355	-1.745791
14	1	0	5.423825	-1.987571	1.012725
15	1	0	4.221349	-1.478959	2.235512
16	1	0	4.105083	-3.083013	1.460663
17	6	0	-2.151193	-2.107396	-0.717195
18	6	0	-2.950954	-0.265180	0.643472
19	6	0	-4.159358	-0.927316	0.817494
20	6	0	-3.373448	-2.759646	-0.526919
21	6	0	-4.390299	-2.187339	0.240176
22	1	0	-4.939541	-0.452180	1.410551
23	1	0	-1.390610	-2.579953	-1.330712
24	1	0	-3.528205	-3.730483	-0.996193
25	1	0	-5.339457	-2.699485	0.380209
26	8	0	-0.933712	2.559459	0.535762
27	8	0	-0.537925	4.770869	0.369208
28	1	0	-2.781888	0.714602	1.082771
29	1	0	-0.733580	0.827506	0.028567
30	6	0	-0.202457	3.447791	0.003306
31	8	0	0.754071	3.336096	-0.780414