Supplementary Data for

Reactions of the hydroperoxide anion with dimethyl methylphosphonate in an ion trap mass spectrometer: evidence for a gas phase α-effect

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Supplementary Table 1 – Vibrational Partition functions for initial transition states for the reaction of HOO^- with DMMP as shown in Figures 8 and 9.

S_N2(carbon) (TS1)		**deprotonation (TS2)**		**addition-elimination (TS3)**	
cm^{-1}	Q'_{vib}	cm^{-1}	Q'_{vib}	cm^{-1}	Q'_{vib}
-420.48		-970.87		-90.24	
19.93	11.29	46.77	5.11	69.04	3.64
28.34	8.10	67.89	3.69	74.94	3.40
50.55	4.77	84.12	3.09	110.96	2.48
82.83	3.13	115.65	2.40	132.35	2.18
113.27	2.44	124.67	2.27	134.68	2.15
122.99	2.30	139.33	2.10	177.93	1.78
136.40	2.13	152.48	1.97	182.88	1.75
167.39	1.85	199.69	1.65	203.61	1.63
176.24	1.79	209.23	1.61	236.09	1.50
221.36	1.56	225.51	1.54	252.08	1.45
250.43	1.45	281.07	1.37	269.09	1.40
256.62	1.43	303.83	1.32	307.25	1.31
287.06	1.36	382.04	1.20	314.50	1.30
299.41	1.33	429.78	1.16	398.03	1.19
369.84	1.22	457.59	1.14	452.24	1.14
436.89	1.15	504.58	1.11	481.95	1.12
463.47	1.13	527.95	1.09	531.97	1.09
507.50	1.10	563.59	1.08	665.01	1.05
691.85	1.04	685.40	1.04	711.84	1.04
757.20	1.03	731.78	1.03	800.37	1.02
850.39	1.02	857.66	1.02	868.39	1.02
890.40	1.02	878.41	1.02	936.91	1.01
914.63	1.01	907.90	1.01	950.27	1.01
955.72	1.01	965.09	1.01	1042.24	1.01
1082.27	1.01	1048.30	1.01	1088.95	1.01
1088.89	1.01	1075.27	1.01	1182.24	1.00
1092.88	1.01	1178.67	1.00	1197.38	1.00
1182.44	1.00	1188.06	1.00	1202.01	1.00
1200.72	1.00	1192.99	1.00	1209.19	1.00
1210.14	1.00	1202.69	1.00	1218.18	1.00
1234.56	1.00	1223.52	1.00	1308.05	1.00
1269.37	1.00	1374.39	1.00	1355.46	1.00
1348.34	1.00	1409.70	1.00	1451.45	1.00
1429.38	1.00	1427.02	1.00	1459.16	1.00
1438.11	1.00	1477.12	1.00	1480.85	1.00
1482.60	1.00	1496.34	1.00	1499.61	1.00
1487.28	1.00	1508.77	1.00	1511.00	1.00
1488.99	1.00	1521.76	1.00	1522.54	1.00
1511.58	1.00	1529.85	1.00	1531.94	1.00
1531.67	1.00	1548.99	1.00	1560.77	1.00
3031.64	1.00	1654.70	1.00	2930.23	1.00

3059.37	1.00	3016.20	1.00	2977.29	1.00
3096.72	1.00	3028.92	1.00	3026.13	1.00
3113.49	1.00	3073.76	1.00	3077.78	1.00
3141.30	1.00	3094.67	1.00	3089.49	1.00
3145.74	1.00	3097.16	1.00	3098.86	1.00
3166.72	1.00	3109.41	1.00	3107.27	1.00
3334.28	1.00	3110.79	1.00	3108.07	1.00
3347.76	1.00	3139.08	1.00	3132.30	1.00
3707.12	1.00	3606.24	1.00	3631.11	1.00
Q_{vib}(TS1)	658154	**Q_{vib}(TS2)**	24046	**Q_{vib}(TS3)**	7582

Relative Arrhenius pre-exponential factors are then determined to be as follows S_N2/deprotonation = 27.4, addition-elimination/deprotonation = 0.3, S_N2/addition-elimination = 86.8.

Supplementary Table 2 – Vibrational Partition functions for initial transition states of the analogous reaction pathways of the CH_3O^- ion with DMMP.

S_N2(carbon) (TS5)		**deprotonation (TS6)**		**addition-elimination (TS7)**	
cm^{-1}	Q'_{vib}	cm^{-1}	Q'_{vib}	cm^{-1}	Q'_{vib}
-434.17		-1019.61		-119.53	
14.96	14.88	23.75	9.56	59.87	4.11
34.47	6.75	46.26	5.16	68.53	3.66
51.25	4.71	75.23	3.39	95.36	2.79
56.09	4.35	87.37	2.99	100.57	2.68
82.87	3.13	106.20	2.57	123.75	2.28
114.99	2.41	127.55	2.23	128.56	2.22
118.09	2.37	127.87	2.23	140.03	2.09
123.37	2.29	146.26	2.03	163.32	1.88
169.81	1.83	188.54	1.71	184.16	1.74
173.84	1.80	199.48	1.65	198.98	1.66
247.91	1.46	218.96	1.57	259.33	1.43
253.14	1.45	280.06	1.37	280.79	1.37
285.63	1.36	311.70	1.31	303.76	1.32
323.70	1.29	384.66	1.20	345.62	1.25
332.37	1.27	426.32	1.16	402.95	1.18
435.16	1.15	483.56	1.12	455.10	1.14
468.31	1.13	517.45	1.10	482.56	1.12
506.09	1.10	543.26	1.09	645.01	1.05
693.50	1.04	685.42	1.04	667.83	1.05
756.73	1.03	722.49	1.04	788.66	1.03
887.86	1.02	864.82	1.02	927.27	1.01
914.81	1.01	893.23	1.02	954.69	1.01
951.83	1.01	975.02	1.01	1071.39	1.01
1078.89	1.01	1054.47	1.01	1100.61	1.01
1082.28	1.01	1079.94	1.01	1134.83	1.01
1104.61	1.01	1123.24	1.01	1179.50	1.00

1141.17	1.00	1170.60	1.00	1180.54	1.00
1179.14	1.00	1180.97	1.00	1182.64	1.00
1181.38	1.00	1187.64	1.00	1188.57	1.00
1182.83	1.00	1195.14	1.00	1204.06	1.00
1202.68	1.00	1198.73	1.00	1205.52	1.00
1210.75	1.00	1205.69	1.00	1216.17	1.00
1271.99	1.00	1221.28	1.00	1309.40	1.00
1347.13	1.00	1379.80	1.00	1427.45	1.00
1422.72	1.00	1427.94	1.00	1459.20	1.00
1427.46	1.00	1477.89	1.00	1476.99	1.00
1480.14	1.00	1493.77	1.00	1479.25	1.00
1482.63	1.00	1497.51	1.00	1486.67	1.00
1483.00	1.00	1498.51	1.00	1497.16	1.00
1486.93	1.00	1508.71	1.00	1501.97	1.00
1489.23	1.00	1515.05	1.00	1507.51	1.00
1497.12	1.00	1524.02	1.00	1512.32	1.00
1511.23	1.00	1530.79	1.00	1532.20	1.00
1530.91	1.00	1547.59	1.00	1549.99	1.00
2636.38	1.00	1635.12	1.00	2659.05	1.00
2676.38	1.00	2845.02	1.00	2744.97	1.00
2763.38	1.00	2862.61	1.00	2826.33	1.00
3033.60	1.00	2873.91	1.00	3009.74	1.00
3059.09	1.00	3017.27	1.00	3021.68	1.00
3099.64	1.00	3024.96	1.00	3042.21	1.00
3116.11	1.00	3064.12	1.00	3067.92	1.00
3140.19	1.00	3088.95	1.00	3087.99	1.00
3146.00	1.00	3094.57	1.00	3097.33	1.00
3172.53	1.00	3102.48	1.00	3121.97	1.00
3337.13	1.00	3106.94	1.00	3126.45	1.00
3349.95	1.00	3126.24	1.00	3156.82	1.00
$\mathbf{Q_{vib}}$	2223861	$\mathbf{Q_{vib}}$	229496	$\mathbf{Q_{vib}}$	38540

Relative Arrhenius pre-exponential factors are then determined to be as follows S_N2/deprotonation = 9.7, addition-elimination/deprotonation = 0.2, S_N2/addition-elimination = 57.7.

Standard orientations for stationary points calculated on the B3LYP/6-31+G(d) potential energy surface

Reactants

HOO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.900800	-0.858933	0.000000
2	8	0	0.056300	-0.706551	0.000000
3	8	0	0.056300	0.813918	0.000000

CH_3O^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.796473	-0.000001	0.000001
2	6	0	-0.543713	-0.000002	0.000002
3	1	0	-1.036484	1.029745	-0.038126
4	1	0	-1.036522	-0.481847	0.910778
5	1	0	-1.036499	-0.547875	-0.872672

DMMP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.001172	0.373713	0.172016
2	8	0	0.927025	-0.637562	-0.708864
3	8	0	0.148677	0.186023	1.642602
4	8	0	-1.466433	0.100865	-0.453744
5	6	0	2.129037	-1.201136	-0.150525
6	6	0	0.329858	2.034722	-0.466476
7	6	0	-2.171391	-1.110986	-0.120925
8	1	0	2.377763	-2.064666	-0.770826
9	1	0	1.967509	-1.509622	0.885455
10	1	0	2.946388	-0.472296	-0.195730
11	1	0	-0.353527	2.746353	0.005617
12	1	0	0.196555	2.061915	-1.551233
13	1	0	1.358045	2.313591	-0.216506
14	1	0	-3.164555	-1.013397	-0.562351
15	1	0	-2.251797	-1.220997	0.964514
16	1	0	-1.657982	-1.976782	-0.551582

Products

P1, product ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.393814	-0.225639	0.000062
2	8	0	-0.413472	-0.967119	-1.323083
3	8	0	-0.412481	-0.966160	1.323762
4	8	0	0.939762	0.835905	-0.000770
5	6	0	2.215338	0.224884	-0.000106
6	1	0	2.359773	-0.400987	-0.893595
7	1	0	2.359372	-0.399841	0.894243
8	1	0	2.966954	1.026030	-0.000473
9	6	0	-1.685804	1.091638	0.000031
10	1	0	-1.599358	1.716812	-0.895525
11	1	0	-1.599042	1.717190	0.895294
12	1	0	-2.668164	0.605233	0.000297

CH_3OOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.133662	-0.223556	0.029435
2	1	0	-1.149910	-0.809417	0.957188
3	1	0	-1.184913	-0.889593	-0.839727
4	1	0	-1.974195	0.478205	0.010726
5	8	0	0.014798	0.607527	-0.036763
6	8	0	1.162339	-0.296156	-0.082196
7	1	0	1.693895	0.071166	0.646875

CH_3OCH_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000024	-0.587578	0.000015
2	6	0	1.177358	0.195665	0.000014
3	1	0	2.023806	-0.495913	-0.001161
4	1	0	1.233290	0.836890	-0.894908
5	1	0	1.234427	0.835302	0.895972
6	6	0	-1.177329	0.195684	-0.000001
7	1	0	-1.233431	0.836627	-0.895101
8	1	0	-2.023725	-0.495961	-0.000776
9	1	0	-1.234349	0.835582	0.895777

P2, product ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.065111	0.503692	0.109856
2	8	0	-0.044932	0.444980	1.618310
3	8	0	0.696268	-0.949993	-0.484961
4	6	0	1.989787	-1.307429	-0.028805
5	1	0	1.981378	-1.536668	1.046733
6	1	0	2.296629	-2.202330	-0.586563
7	1	0	2.706294	-0.494519	-0.212750
8	8	0	-1.448063	0.233039	-0.580935
9	6	0	-2.223548	-0.858887	-0.104297
10	1	0	-2.290692	-0.846445	0.991599
11	1	0	-1.794407	-1.819311	-0.424116
12	1	0	-3.229747	-0.754101	-0.531873
13	6	0	0.889541	1.784159	-0.625320
14	1	0	0.890796	2.728845	-0.086795
15	1	0	0.902223	1.837876	-1.712851

HOOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.728286	-0.054469
2	1	0	0.823819	0.901515	0.435749
3	8	0	0.000000	-0.728286	-0.054469
4	1	0	-0.823819	-0.901515	0.435749

P3, product ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.004294	0.442851	0.120203
2	8	0	0.324919	-0.015427	1.532650
3	8	0	-0.948597	-0.677983	-0.673386
4	6	0	-2.133953	-1.105754	-0.016935
5	1	0	-1.905559	-1.542591	0.964210
6	1	0	-2.835333	-0.270772	0.120107
7	1	0	-2.595512	-1.867850	-0.656584
8	6	0	-0.659560	1.960223	-0.200459
9	1	0	-0.241693	2.821413	0.314632
10	1	0	-1.107069	2.129703	-1.176522
11	8	0	1.426479	0.195610	-0.742023
12	8	0	2.154897	-1.012658	-0.215692
13	1	0	1.849077	-0.955821	0.723083

P4, product ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.452907	-0.032120	0.176640
2	8	0	-0.423740	-0.268675	1.658569
3	8	0	0.629372	-0.978536	-0.627092
4	6	0	1.975253	-1.058186	-0.145056
5	1	0	2.471212	-0.095114	-0.293869
6	1	0	1.985846	-1.316192	0.921072
7	1	0	2.462385	-1.853070	-0.723478
8	6	0	-1.996521	-0.649691	-0.599195
9	1	0	-2.832166	-0.022445	-0.271433
10	1	0	-2.177935	-1.680016	-0.277260
11	1	0	-1.925980	-0.612274	-1.690863
12	8	0	-0.385396	1.435962	-0.424405
13	8	0	1.046996	1.849770	-0.088104

CH_3OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.749567	0.122899	-0.000031
2	6	0	-0.668897	-0.020937	-0.000009
3	1	0	-1.080878	0.991433	-0.001819
4	1	0	-1.029494	-0.544763	0.896794
5	1	0	-1.029320	-0.548157	-0.894912
6	1	0	1.156535	-0.756086	0.000237

P5, product ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.444693	0.266530	-0.480923
2	8	0	-0.592258	1.524779	0.405636
3	8	0	0.876911	-0.715522	0.190487
4	6	0	-1.703240	-0.984701	0.190980
5	6	0	2.155079	-0.149392	0.048594
6	1	0	-1.590678	-1.064869	1.281573
7	1	0	-1.563222	-1.973158	-0.268748
8	1	0	-2.713313	-0.619655	-0.039997
9	1	0	2.899191	-0.878972	0.402902
10	1	0	2.263842	0.775439	0.638524
11	1	0	2.386328	0.093762	-1.006838

CH_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.677849
2	6	0	0.000000	0.000000	-0.531557
3	1	0	0.000000	0.941506	-1.116728
4	1	0	0.000000	-0.941506	-1.116728

Ion Complexes and Intermediates

RC1, reactant complex with HOO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.722790	-0.265018	0.164417
2	8	0	0.844082	-0.287861	1.657436
3	8	0	0.544019	1.230977	-0.456852
4	6	0	-0.545618	2.058950	0.032121
5	1	0	-0.338785	2.355180	1.067352
6	1	0	-0.550599	2.943078	-0.611809
7	1	0	-1.508686	1.525181	-0.035766
8	8	0	2.113698	-0.693825	-0.603999
9	6	0	3.338461	-0.107824	-0.159024
10	1	0	3.463873	-0.239164	0.921864
11	1	0	3.367288	0.961406	-0.402632
12	1	0	4.143651	-0.624238	-0.690701
13	6	0	-0.522806	-1.309632	-0.590812
14	1	0	-0.580440	-2.258420	-0.048750
15	1	0	-0.259258	-1.491670	-1.638040
16	1	0	-1.518338	-0.774758	-0.554026
17	8	0	-3.031328	0.263684	-0.510219
18	8	0	-3.829396	-0.752125	0.250647
19	1	0	-3.809367	-0.357089	1.136437

RC2, reactant complex with CH_3O^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.787297	-0.267036	0.194976
2	8	0	0.959295	-0.214146	1.682109
3	8	0	0.507489	1.176841	-0.495372
4	6	0	-0.613791	1.982005	-0.028615
5	1	0	-0.430391	2.286376	1.008616
6	1	0	-0.619563	2.863882	-0.676199
7	1	0	-1.562315	1.423302	-0.118002
8	8	0	2.174733	-0.665132	-0.598725
9	6	0	3.378819	0.008447	-0.228499
10	1	0	3.539527	-0.045968	0.854401
11	1	0	3.346279	1.059875	-0.540030
12	1	0	4.195626	-0.500431	-0.749867
13	6	0	-0.411266	-1.430589	-0.460191
14	1	0	-0.360797	-2.359232	0.117800
15	1	0	-0.185589	-1.633802	-1.512251
16	1	0	-1.440444	-0.970396	-0.393500
17	8	0	-2.957356	0.041244	-0.439825
18	6	0	-4.081749	-0.413192	0.174964
19	1	0	-4.451094	0.241438	1.014543
20	1	0	-3.973927	-1.432618	0.646642
21	1	0	-4.972135	-0.517361	-0.508246

PC1, product ion complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.937805	-0.439027	-0.029775
2	8	0	-0.101940	0.452898	0.886986
3	8	0	-1.960157	0.564689	-0.910178
4	6	0	-2.364808	1.802925	-0.348959
5	1	0	-3.101656	1.660753	0.459331
6	1	0	-1.509502	2.356260	0.055057
7	1	0	-2.838459	2.382874	-1.151020
8	8	0	-0.302300	-1.389550	-1.011366
9	6	0	3.099568	-0.493419	-0.823900
10	1	0	2.090190	-0.905949	-0.941862
11	1	0	3.521459	-0.252653	-1.809294
12	1	0	3.752501	-1.214447	-0.309049
13	6	0	-2.151462	-1.350376	1.018871
14	1	0	-1.603253	-2.039836	1.670823
15	1	0	-2.835483	-1.927493	0.387131
16	1	0	-2.727807	-0.662771	1.649491
17	8	0	3.081433	0.748601	-0.130318
18	8	0	2.564261	0.488846	1.203580
19	1	0	1.568927	0.510014	1.050323

PC2, product ion complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.473362	-0.203824	0.278622
2	8	0	0.035621	-0.734453	-1.052754
3	8	0	-0.828331	1.419032	0.168774
4	6	0	0.162998	2.280469	-0.390595
5	1	0	0.406990	1.980403	-1.416728
6	1	0	-0.264114	3.289968	-0.392406
7	1	0	1.081977	2.267181	0.206151
8	8	0	-2.046874	-0.710064	0.496021
9	6	0	-2.948671	-0.628154	-0.605894
10	1	0	-2.544967	-1.151168	-1.481141
11	1	0	-3.147826	0.418696	-0.872271
12	1	0	-3.883981	-1.104578	-0.289026
13	6	0	0.533759	-0.429955	1.640566
14	1	0	0.815123	-1.472219	1.807769
15	1	0	0.206670	0.085197	2.545796
16	1	0	2.238833	-0.026740	0.802317
17	8	0	3.007252	0.101811	0.151488
18	8	0	2.812783	-1.031707	-0.756327
19	1	0	1.859602	-0.920494	-1.011870

INT1, pentavalent intermediate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.161251	-0.335752	-0.046891
2	8	0	0.131181	-0.536314	1.476110
3	8	0	0.041849	1.224449	-0.655538
4	6	0	-1.166094	1.977740	-0.635045
5	1	0	-1.647528	1.954073	0.347505
6	1	0	-0.878611	3.007747	-0.886185
7	1	0	-1.884994	1.603479	-1.372618
8	8	0	1.903210	-0.205459	-0.238110
9	6	0	2.626659	0.594565	0.665559
10	1	0	2.469251	0.274229	1.705153
11	1	0	2.345865	1.658025	0.583281
12	1	0	3.694671	0.499362	0.415067
13	6	0	0.230033	-1.630433	-1.376723
14	1	0	0.331171	-2.600730	-0.877070
15	1	0	1.100674	-1.462851	-2.013824
16	1	0	-0.695305	-1.637314	-1.957134
17	8	0	-1.671968	-0.624401	-0.213141
18	8	0	-2.378068	-0.292086	1.029902
19	1	0	-1.607182	-0.440478	1.642650

PC3, product ion complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.636906	-0.247277	-0.159020
2	8	0	-0.525911	-0.505849	1.332210
3	8	0	-0.739979	1.369784	-0.488284
4	6	0	0.194601	2.242885	0.147282
5	1	0	0.121623	2.161526	1.238793
6	1	0	1.223002	2.019980	-0.163241
7	1	0	-0.070118	3.260004	-0.162076
8	8	0	3.168385	-0.026025	-0.476923
9	6	0	3.408045	-0.615242	0.784419
10	1	0	2.525768	-0.559044	1.439169
11	1	0	4.237555	-0.076853	1.263695
12	1	0	3.700839	-1.678153	0.700216
13	6	0	0.493511	-0.909754	-1.250460
14	1	0	0.606103	-1.993521	-1.186833
15	1	0	2.240013	-0.304357	-0.768327
16	1	0	0.412563	-0.531193	-2.270593
17	8	0	-2.205152	-0.708212	-0.568239
18	8	0	-3.137118	-0.422961	0.563250
19	1	0	-2.502506	-0.550461	1.310948

Transitions States

TS1, S_N2(carbon) process

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.123375	0.324776	0.197054
2	8	0	-1.260305	0.219184	1.688095
3	8	0	-0.043728	-0.562222	-0.514836
4	6	0	1.600479	-0.613539	-0.009081
5	1	0	1.976493	0.279520	-0.486450
6	1	0	1.496433	-0.609890	1.066109
7	1	0	1.833477	-1.554939	-0.479414
8	8	0	-2.527115	-0.056737	-0.597101
9	6	0	-3.075352	-1.355352	-0.375068
10	1	0	-3.239695	-1.533304	0.694763
11	1	0	-2.411410	-2.131642	-0.775541
12	1	0	-4.033821	-1.388204	-0.903188
13	6	0	-0.930187	2.045238	-0.379185
14	1	0	-1.734828	2.667564	0.024714
15	1	0	-0.940989	2.088574	-1.472447
16	1	0	0.030365	2.424843	-0.015424
17	8	0	3.747498	-0.674521	0.470480
18	8	0	4.282445	0.395304	-0.413094
19	1	0	4.714586	-0.140302	-1.097283

TS2, deprotonation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.517542	-0.285565	-0.088080
2	8	0	0.211666	-0.495734	1.372823
3	8	0	0.603640	1.318254	-0.467780
4	6	0	-0.417345	2.190152	0.055048
5	1	0	-0.276226	2.327664	1.133823
6	1	0	-0.288061	3.149166	-0.457948
7	1	0	-1.419706	1.785541	-0.136301
8	8	0	2.080597	-0.686773	-0.457163
9	6	0	3.120519	-0.223490	0.405180
10	1	0	2.921150	-0.509036	1.444685
11	1	0	3.221894	0.867625	0.341343
12	1	0	4.048081	-0.695085	0.063149
13	6	0	-0.577029	-1.029079	-1.232003
14	1	0	-0.627488	-2.111739	-1.075776
15	1	0	-0.307451	-0.791996	-2.266539
16	1	0	-1.804720	-0.517039	-0.912899
17	8	0	-2.877752	0.011040	-0.461381
18	8	0	-3.003371	-0.681057	0.838973
19	1	0	-2.105699	-0.572968	1.214535

TS3, 1st transition state for addition-elimination

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.445964	-0.322028	-0.027261
2	8	0	0.028901	-0.327874	1.413486
3	8	0	0.314531	1.097768	-0.804222
4	6	0	-0.775176	2.019507	-0.526456
5	1	0	-0.605876	2.492010	0.448085
6	1	0	-0.719155	2.773092	-1.319319
7	1	0	-1.720020	1.448425	-0.544046
8	8	0	2.095010	-0.494597	-0.163336
9	6	0	2.923961	0.375516	0.601005
10	1	0	2.657124	0.338674	1.664255
11	1	0	2.841117	1.410001	0.242134
12	1	0	3.954901	0.029443	0.469684
13	6	0	-0.039128	-1.697829	-1.096527
14	1	0	0.383322	-2.623182	-0.689305
15	1	0	0.345196	-1.532792	-2.108359
16	1	0	-1.139989	-1.702326	-1.067090
17	8	0	-2.442728	-0.323495	-0.426482
18	8	0	-2.906798	-0.164330	0.980693
19	1	0	-2.055344	-0.285867	1.443633

TS4, 2nd transition state for addition-elimination

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.508856	-0.253514	-0.057434
2	8	0	-0.359381	-0.252832	1.437729
3	8	0	-0.282596	1.146758	-0.822762
4	6	0	0.712774	2.105237	-0.386339
5	1	0	0.428256	2.504949	0.593478
6	1	0	1.682149	1.586383	-0.352573
7	1	0	0.686283	2.903985	-1.134305
8	8	0	2.345114	-0.254391	-0.324017
9	6	0	3.172228	-0.396169	0.753250
10	1	0	2.893058	-1.239563	1.437513
11	1	0	3.209514	0.507562	1.422346
12	1	0	4.243457	-0.587515	0.473454
13	6	0	0.036808	-1.623662	-1.100394
14	1	0	-0.262318	-2.564122	-0.627437
15	1	0	1.134179	-1.518831	-1.142868
16	1	0	-0.434963	-1.537960	-2.085445
17	8	0	-2.169700	-0.471813	-0.341461
18	8	0	-2.927910	0.226247	0.701566
19	1	0	-2.321850	0.083639	1.469818

TS5, S_N2(carbon) process (with CH_3O^-)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.201603	0.357119	0.147878
2	8	0	-1.319731	0.442539	1.641011
3	8	0	0.000202	-0.450256	-0.458345
4	6	0	1.616279	-0.269931	0.067163
5	1	0	1.890468	0.621381	-0.476998
6	1	0	1.501525	-0.186811	1.137132
7	1	0	1.970650	-1.211784	-0.320454
8	8	0	-2.528296	-0.332848	-0.562064
9	6	0	-2.858887	-1.668669	-0.181304
10	1	0	-3.001097	-1.742489	0.903792
11	1	0	-2.073236	-2.367055	-0.494595
12	1	0	-3.794717	-1.919187	-0.690914
13	6	0	-1.268431	1.990766	-0.663696
14	1	0	-2.168325	2.527327	-0.347267
15	1	0	-1.265875	1.881795	-1.752420
16	1	0	-0.387880	2.565256	-0.357372
17	8	0	3.739804	-0.098608	0.650758
18	6	0	4.500214	-0.242188	-0.465422
19	1	0	4.375117	-1.233010	-0.993933
20	1	0	5.601128	-0.167677	-0.267965
21	1	0	4.305421	0.528983	-1.268506

TS6, deprotonation (with CH_3O^-)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.673220	-0.305715	0.134835
2	8	0	0.763564	-0.315396	1.636408
3	8	0	0.639314	1.233400	-0.470258
4	6	0	-0.381117	2.122173	0.015103
5	1	0	-0.246149	2.302381	1.089198
6	1	0	-0.251125	3.062392	-0.532168
7	1	0	-1.381041	1.711174	-0.173458
8	8	0	2.108110	-0.755243	-0.572204
9	6	0	3.312247	-0.164206	-0.088220
10	1	0	3.392771	-0.273328	1.000225
11	1	0	3.356785	0.901425	-0.348749
12	1	0	4.141895	-0.690986	-0.573091
13	6	0	-0.621925	-1.201372	-0.632477
14	1	0	-0.727163	-2.180647	-0.152541
15	1	0	-0.420556	-1.324000	-1.703079
16	1	0	-1.834894	-0.527079	-0.581305
17	8	0	-2.935375	0.057614	-0.607075
18	6	0	-3.758604	-0.467702	0.375208
19	1	0	-3.252587	-1.256150	0.976461
20	1	0	-4.680420	-0.935161	-0.040120
21	1	0	-4.104325	0.299347	1.103438

TS7, addition-elimination (with CH_3O^-)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.416924	-0.324505	0.023412
2	8	0	0.146241	-0.284407	1.496179
3	8	0	0.273794	1.077966	-0.805234
4	6	0	-0.776868	2.023691	-0.537587
5	1	0	-0.747868	2.330583	0.514495
6	1	0	-0.561905	2.885486	-1.180716
7	1	0	-1.737008	1.548090	-0.761728
8	8	0	2.085901	-0.455865	-0.196568
9	6	0	2.922108	0.413255	0.549282
10	1	0	2.712400	0.339518	1.624198
11	1	0	2.793296	1.458202	0.231185
12	1	0	3.958397	0.109023	0.357100
13	6	0	0.047501	-1.764300	-1.028199
14	1	0	0.361967	-2.659712	-0.480399
15	1	0	0.633037	-1.686261	-1.950307
16	1	0	-1.030307	-1.771677	-1.204685
17	8	0	-2.199919	-0.378649	-0.346038
18	6	0	-3.043826	-0.178795	0.709120
19	1	0	-2.642709	-0.555118	1.680162
20	1	0	-3.292086	0.906600	0.901818
21	1	0	-4.042696	-0.672625	0.575290