Electronic Supplementary Material for PCCP

Supporting Information:

Thermochemistry and Kinetics of Acetonylperoxy Radical Isomerisation and Decomposition: A Quantum Chemistry and CVT/SCT Approach

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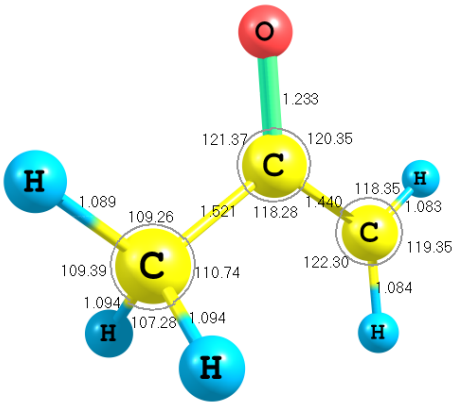
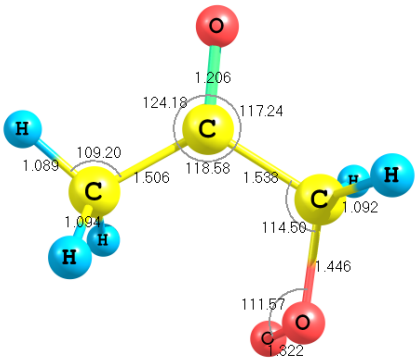
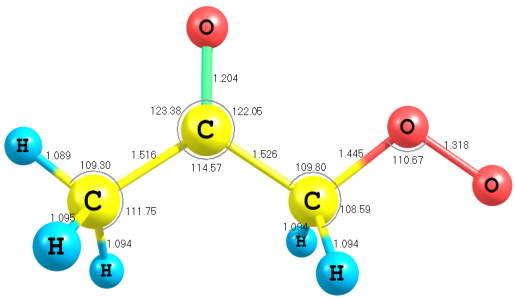


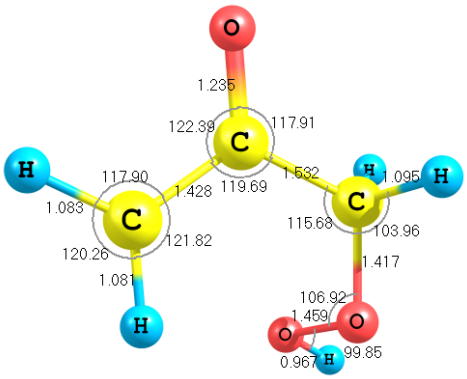
$H_3CC(O)CH_2$•



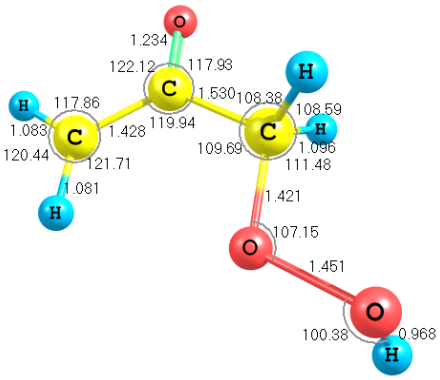
$CH_3C(O)CH_2OO$•,syn



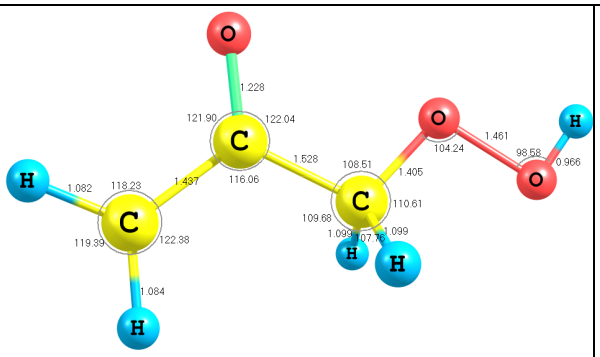
$CH_3C(O)CH_2O_2$•, anti



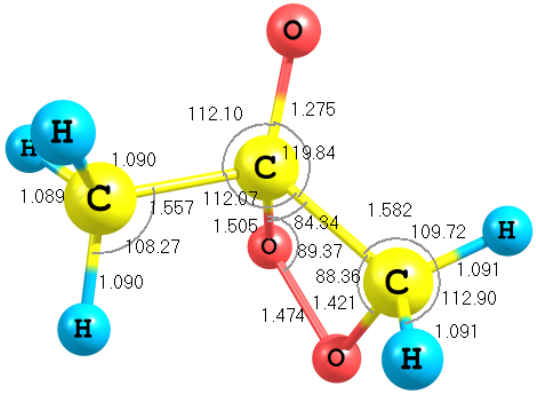
$H_2C•C(O)CH_2OOH$, syn



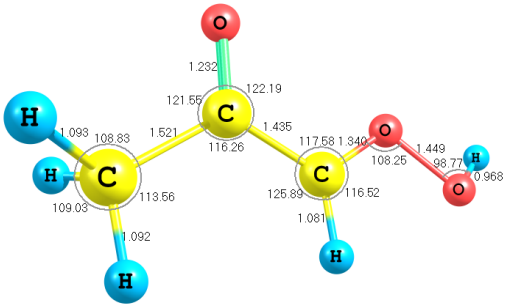
$C•H_2COCH_2O_2H$, anti



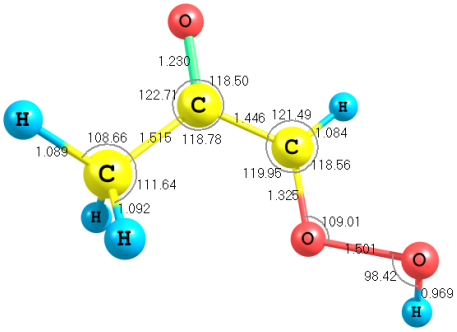
$H_2C•C(O)CH_2OOH$, anti



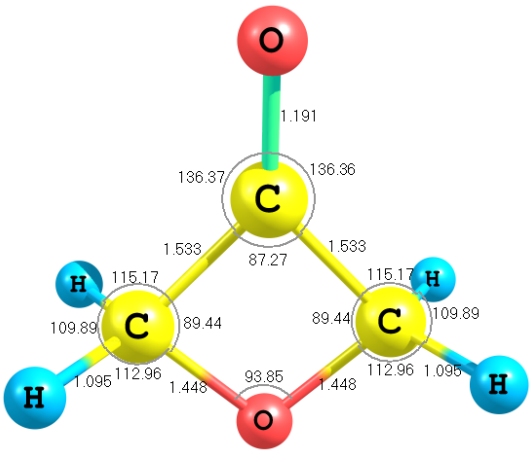
Cyclic acetonyl peroxy radical



$CH_3C(O)C•HO_2H$, anti



$CH_3C(O)C•HOOH$



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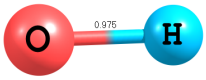
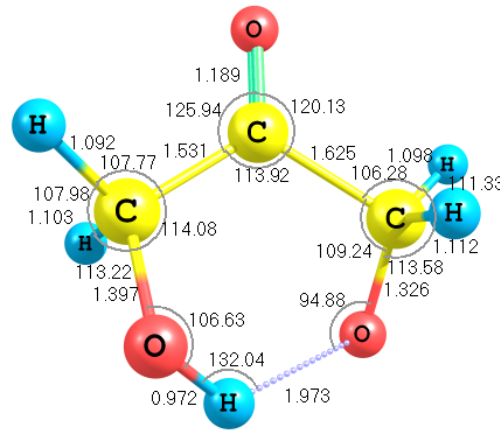
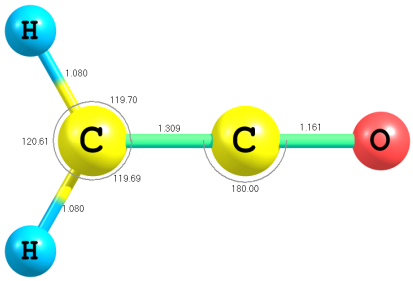


Oxetan-3-one + OH



$CH_2OHC(O)CH_2O•$



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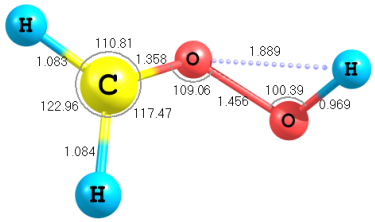
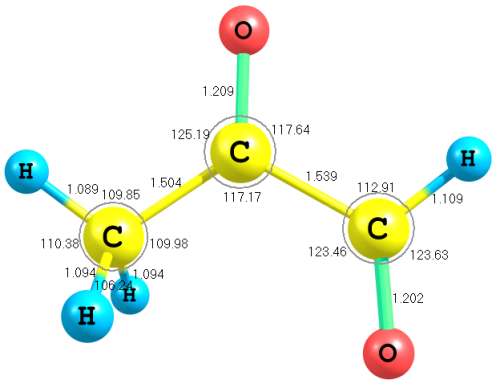
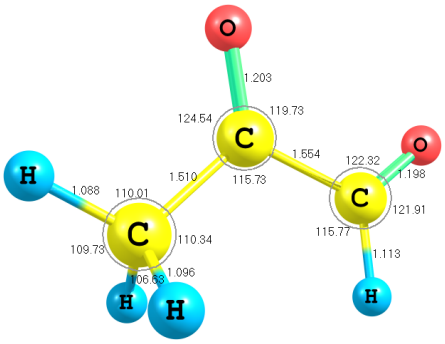


$H_2C=C=O + H_2C•OOH$



$CH_3C(O)CHO$, syn



$CH_3C(O)CHO$, anti

CH_3COCH_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.358903	-0.355810	-0.000025
2	6	0	0.085852	0.119240	-0.000013
3	8	0	0.366689	1.319431	-0.000007
4	6	0	1.129681	-0.872035	-0.000004
5	1	0	-2.021258	0.508555	-0.002124
6	1	0	-1.564283	-0.972915	-0.880016
7	1	0	-1.565222	-0.969117	0.882419
8	1	0	2.158636	-0.535058	0.000095
9	1	0	0.918835	-1.935279	-0.000066

Frequencies --	50.5874	364.9956	386.0310
Frequencies --	507.7708	526.7403	750.3779
Frequencies --	814.3581	923.6945	1025.2335
Frequencies --	1064.6360	1264.0291	1389.0840
Frequencies --	1455.2980	1473.8146	1478.9313
Frequencies --	1593.2377	3029.8059	3085.9553
Frequencies --	3138.3932	3140.6105	3254.8587

Rotational constants (GHZ): 10.95642 9.04637 5.11201

Zero-point correction= 0.069982 (Hartree/Particle)
Thermal correction to Energy= 0.075060

Thermal correction to Enthalpy= 0.076004
Thermal correction to Gibbs Free Energy= 0.041623

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.069282 E(Thermal)= 0.074388
E(SCF)= -191.409036 DE(MP2)= -0.678429
DE(CBS)= -0.068926 DE(MP34)= -0.044198
DE(CCSD)= -0.023638 DE(Int)= 0.022236
DE(Empirical)= -0.035723
CBS-QB3 (0 K)= -192.168433 CBS-QB3 Energy= -192.163326
CBS-QB3 Enthalpy= -192.162382 CBS-QB3 Free Energy= -192.196814

$CH_3COCH_2O_2$, O_2 syn w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.264172	-0.961932	0.160785
2	6	0	0.990964	-0.089776	-0.011401
3	6	0	0.864478	1.399681	0.173741
4	1	0	-0.105426	-1.648867	0.994028
5	1	0	-0.442130	-1.522058	-0.757985
6	8	0	-1.463494	-0.227196	0.496279
7	8	0	-1.990891	0.354153	-0.567533
8	8	0	2.022105	-0.653722	-0.282690
9	1	0	1.847279	1.857312	0.075729
10	1	0	0.431900	1.626942	1.152633
11	1	0	0.178991	1.812952	-0.571597

Frequencies -- 45.4945 106.0867 169.1817
Frequencies -- 247.1889 394.1305 464.8213
Frequencies -- 492.7791 574.7581 757.8166
Frequencies -- 859.4883 943.6111 991.7741
Frequencies -- 1091.6505 1154.0308 1222.5556
Frequencies -- 1273.9280 1332.6097 1388.7112
Frequencies -- 1433.1574 1461.7713 1468.1457
Frequencies -- 1809.5866 3037.4335 3074.2623
Frequencies -- 3094.7013 3136.9780 3150.4718

Rotational constants (GHZ): 6.93034 2.48994 2.04323

Zero-point correction= 0.080139 (Hartree/Particle)

Thermal correction to Energy= 0.086959
Thermal correction to Enthalpy= 0.087904
Thermal correction to Gibbs Free Energy= 0.048133

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.079338 E(Thermal)= 0.086196
E(SCF)= -341.088240 DE(MP2)= -1.146079
DE(CBS)= -0.116538 DE(MP34)= -0.047395
DE(CCSD)= -0.034893 DE(Int)= 0.036031
DE(Empirical)= -0.055089
CBS-QB3 (0 K)= -342.372865 CBS-QB3 Energy= -342.366007
CBS-QB3 Enthalpy= -342.365063 CBS-QB3 Free Energy= -342.404911

$CH_3COCH_2O_2$, O_2 anti w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.211837	-0.717719	0.032456
2	6	0	-0.988511	0.175513	-0.020093
3	8	0	-1.046184	1.377799	-0.027351
4	6	0	0.341096	-0.571388	-0.058414
5	1	0	-3.098766	-0.127046	-0.192148
6	1	0	-2.131780	-1.556238	-0.665212
7	1	0	-2.311564	-1.139594	1.038313
8	8	0	1.432948	0.365366	0.081182
9	1	0	0.406671	-1.306419	0.749196
10	1	0	0.454622	-1.095009	-1.012704
11	8	0	2.592777	-0.254931	-0.008973

Frequencies -- 34.7103 67.7619 92.3431
Frequencies -- 185.5191 357.5226 443.4492
Frequencies -- 467.9754 591.2747 835.2756
Frequencies -- 855.2656 921.7130 1037.9331
Frequencies -- 1075.2004 1178.8365 1189.4547
Frequencies -- 1229.6509 1373.1903 1389.3297
Frequencies -- 1453.4593 1464.7642 1475.7629
Frequencies -- 1823.5891 3028.5237 3041.0609
Frequencies -- 3084.1517 3090.6888 3143.0526

Rotational constants (GHZ): 9.43132 1.99963 1.68666

Zero-point correction= 0.079580 (Hartree/Particle)

Thermal correction to Energy= 0.086774
Thermal correction to Enthalpy= 0.087718
Thermal correction to Gibbs Free Energy= 0.046337

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.078784 E(Thermal)= 0.086013
E(SCF)= -341.084296 DE(MP2)= -1.145830
DE(CBS)= -0.116416 DE(MP34)= -0.047391
DE(CCSD)= -0.034566 DE(Int)= 0.036024
DE(Empirical)= -0.055075
CBS-QB3 (0 K)= -342.368766 CBS-QB3 Energy= -342.361536
CBS-QB3 Enthalpy= -342.360592 CBS-QB3 Free Energy= -342.402052

CH_2COCH_2OOH, O_2 syn w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.931410	1.369628	0.276900
2	6	0	1.026512	-0.028951	0.004145
3	8	0	2.069512	-0.555578	-0.395230
4	6	0	-0.190474	-0.931048	0.232605
5	1	0	0.007485	1.824720	0.605107
6	1	0	1.813745	1.977367	0.120893
7	1	0	0.014590	-1.569689	1.098427
8	8	0	-1.392542	-0.264829	0.576499
9	1	0	-0.327774	-1.568985	-0.645901
10	8	0	-1.851405	0.428712	-0.622209
11	1	0	-2.717259	0.012379	-0.732901

Frequencies -- 60.5285 128.0321 169.4016
Frequencies -- 272.8194 383.2109 402.0413
Frequencies -- 481.5132 500.7264 567.0692
Frequencies -- 781.1592 818.3405 868.9946
Frequencies -- 996.3439 1013.1624 1063.5484
Frequencies -- 1265.4193 1288.8368 1347.3523
Frequencies -- 1378.1004 1434.9832 1461.3493
Frequencies -- 1563.2615 3035.1023 3086.0806
Frequencies -- 3157.3152 3277.2304 3774.9062

Rotational constants (GHZ): 7.00361 2.44229 2.08052

Zero-point correction= 0.078772 (Hartree/Particle)
Thermal correction to Energy= 0.085816
Thermal correction to Enthalpy= 0.086761
Thermal correction to Gibbs Free Energy= 0.047033

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.077984 E(Thermal)= 0.085072
E(SCF)= -341.069440 DE(MP2)= -1.147866
DE(CBS)= -0.116824 DE(MP34)= -0.047633
DE(CCSD)= -0.035903 DE(Int)= 0.035721
DE(Empirical)= -0.056374
CBS-QB3 (0 K)= -342.360335 CBS-QB3 Energy= -342.353248
CBS-QB3 Enthalpy= -342.352304 CBS-QB3 Free Energy= -342.392117

CH_2COCH_2OOH , O_2 anti w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.271609	-0.635371	0.060844
2	1	0	-0.438712	-1.075876	1.050045
3	1	0	-0.377859	-1.422020	-0.694361
4	6	0	1.159732	-0.098200	0.007623
5	6	0	1.394608	1.309702	0.047595
6	1	0	2.421280	1.652418	0.016804
7	1	0	0.581365	2.020158	0.105652
8	8	0	-1.189789	0.426156	-0.160722
9	8	0	-2.513285	-0.080225	0.153560
10	1	0	-2.916831	-0.070926	-0.725761
11	8	0	2.082371	-0.915999	-0.048932

Frequencies -- 57.8256 88.0971 198.7323
Frequencies -- 203.1688 371.9888 412.6114
Frequencies -- 453.7272 511.5033 530.6775
Frequencies -- 792.9154 844.0007 929.5200
Frequencies -- 1000.0822 1015.4710 1080.4015
Frequencies -- 1225.5353 1278.1128 1356.4863
Frequencies -- 1377.6508 1455.5616 1495.2930
Frequencies -- 1559.7337 3019.2347 3061.5509
Frequencies -- 3153.7097 3274.1377 3764.7742

Rotational constants (GHZ): 9.21322 2.00710 1.68121

Zero-point correction= 0.078625 (Hartree/Particle)
Thermal correction to Energy= 0.085819
Thermal correction to Enthalpy= 0.086763
Thermal correction to Gibbs Free Energy= 0.046443

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.077839 E(Thermal)= 0.085075
E(SCF)= -341.068307 DE(MP2)= -1.145903
DE(CBS)= -0.116757 DE(MP34)= -0.047967
DE(CCSD)= -0.035952 DE(Int)= 0.035667
DE(Empirical)= -0.056433
CBS-QB3 (0 K)= -342.357813 CBS-QB3 Energy= -342.350578
CBS-QB3 Enthalpy= -342.349633 CBS-QB3 Free Energy= -342.390040

$CH_3COCHOOH$, O_2 syn w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.431173	1.282525	-0.084873
2	6	0	-1.090085	-0.191636	-0.009085
3	8	0	-1.944383	-1.074862	-0.060183
4	6	0	0.293191	-0.578532	0.153994
5	1	0	-0.722494	1.828231	-0.711516
6	1	0	-2.442417	1.386641	-0.476228
7	1	0	-1.393362	1.727682	0.914600
8	8	0	1.223922	0.348993	0.322306
9	1	0	0.594552	-1.619589	0.146634
10	8	0	2.496352	-0.111919	-0.326552
11	1	0	3.124993	0.305193	0.281725

Frequencies -- 50.9866 65.5252 153.1139
Frequencies -- 201.3940 239.1402 353.2037
Frequencies -- 466.6348 515.4058 522.2623
Frequencies -- 662.9357 738.6406 828.1955
Frequencies -- 1008.6071 1031.5141 1179.3362
Frequencies -- 1259.8220 1362.6040 1375.3169
Frequencies -- 1394.8501 1467.7043 1476.7675
Frequencies -- 1633.7024 3034.9391 3096.4262
Frequencies -- 3141.5062 3191.1216 3766.6780

Rotational constants (GHZ): 8.29380 2.03449 1.69359

Zero-point correction= 0.077955 (Hartree/Particle)
Thermal correction to Energy= 0.085586
Thermal correction to Enthalpy= 0.086530
Thermal correction to Gibbs Free Energy= 0.044972

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.077176 E(Thermal)= 0.084847
E(SCF)= -341.072517 DE(MP2)= -1.146278
DE(CBS)= -0.117563 DE(MP34)= -0.050789
DE(CCSD)= -0.043317 DE(Int)= 0.035599
DE(Empirical)= -0.056892
CBS-QB3 (0 K)= -342.374583 CBS-QB3 Energy= -342.366911
CBS-QB3 Enthalpy= -342.365967 CBS-QB3 Free Energy= -342.407614

$CH_3COCHOOH$, O_2 anti w.r.t CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.192329	-0.830501	-0.000011
2	6	0	1.025424	0.145380	-0.004888
3	8	0	1.204421	1.363742	-0.028676
4	6	0	-0.286683	-0.433931	0.027946
5	1	0	1.885296	-1.878260	-0.021397
6	1	0	2.825649	-0.627096	-0.866742
7	1	0	2.796624	-0.657991	0.894345
8	8	0	-1.333394	0.401989	0.058955
9	1	0	-0.512601	-1.491178	0.041617
10	8	0	-2.544920	-0.382612	-0.072323
11	1	0	-3.190252	0.303891	0.150253

Frequencies -- 42.2614 67.2704 133.9932
Frequencies -- 180.5682 204.7650 364.4272
Frequencies -- 437.7449 537.8380 595.4010
Frequencies -- 615.3897 902.8064 955.4228
Frequencies -- 1002.7465 1024.5612 1184.9873
Frequencies -- 1234.1269 1394.2762 1448.2304
Frequencies -- 1453.2674 1470.5866 1493.4319
Frequencies -- 1602.3916 3035.4877 3102.0088

Frequencies -- 3112.5900 3217.5731 3780.6777

ROTATIONAL CONSTANTS (GHZ) 9.45490 1.95571 1.63890

Zero-point correction= 0.078810 (Hartree/Particle)
Thermal correction to Energy= 0.086476
Thermal correction to Enthalpy= 0.087420
Thermal correction to Gibbs Free Energy= 0.045523

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.078022 E(Thermal)= 0.085726
E(SCF)= -341.073182 DE(MP2)= -1.155329
DE(CBS)= -0.117624 DE(MP34)= -0.046116
DE(CCSD)= -0.036938 DE(Int)= 0.035820
DE(Empirical)= -0.056204
CBS-QB3 (0 K)= -342.371550 CBS-QB3 Energy= -342.363846
CBS-QB3 Enthalpy= -342.362902 CBS-QB3 Free Energy= -342.404887

CH_3COCHO, CO anti wrt CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.694533	-0.632814	0.000010
2	6	0	-0.430338	0.192932	-0.000046
3	8	0	-0.401246	1.395825	0.000009
4	6	0	0.900175	-0.610107	-0.000031
5	1	0	-2.565593	0.019822	-0.000201
6	1	0	-1.722233	-1.286916	-0.878389
7	1	0	-1.722378	-1.286492	0.878724
8	8	0	1.971471	-0.074348	0.000022
9	1	0	0.796582	-1.718298	0.000027

Frequencies -- 73.3955 123.8341 261.2009
Frequencies -- 401.1952 464.4608 636.4967
Frequencies -- 800.5795 877.0822 966.7856
Frequencies -- 1074.2710 1175.5536 1385.1355
Frequencies -- 1403.0699 1459.6041 1468.2155
Frequencies -- 1804.7438 1836.9184 2866.4996

Frequencies -- 3023.5982 3075.1399 3147.6894

Rotational constants (GHZ): 10.43079 4.01975 2.95434

Zero-point correction= 0.064530 (Hartree/Particle)
Thermal correction to Energy= 0.070266
Thermal correction to Enthalpy= 0.071210
Thermal correction to Gibbs Free Energy= 0.035284

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.063885 E(Thermal)= 0.069648
E(SCF)= -265.722679 DE(MP2)= -0.932193
DE(CBS)= -0.091519 DE(MP34)= -0.031338
DE(CCSD)= -0.025044 DE(Int)= 0.029620
DE(Empirical)= -0.044267
CBS-QB3 (0 K)= -266.753536 CBS-QB3 Energy= -266.747772
CBS-QB3 Enthalpy= -266.746828 CBS-QB3 Free Energy= -266.782812

CH_3COCHO, CO syn wrt CH_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.872247	1.280496	-0.000075
2	6	0	-0.524298	-0.182837	-0.000025
3	8	0	-1.324306	-1.089265	0.000129
4	6	0	0.970440	-0.549731	-0.000171
5	1	0	-1.953926	1.403209	-0.000512
6	1	0	-0.434023	1.768804	0.875090
7	1	0	-0.433204	1.768992	-0.874711
8	8	0	1.853246	0.266315	0.000165
9	1	0	1.146263	-1.644973	-0.000592

Frequencies -- 72.2098 133.5211 247.3088
Frequencies -- 470.1484 482.7316 570.4978
Frequencies -- 775.5839 906.3790 1007.5354
Frequencies -- 1077.8517 1237.5220 1353.6303
Frequencies -- 1390.8797 1457.7847 1461.1755
Frequencies -- 1796.3552 1809.2736 2921.8833
Frequencies -- 3040.0513 3095.0760 3150.8438

Rotational constants (GHZ): 9.09391 4.41659 3.02776

Zero-point correction= 0.064833 (Hartree/Particle)
Thermal correction to Energy= 0.070525
Thermal correction to Enthalpy= 0.071470
Thermal correction to Gibbs Free Energy= 0.035627

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.064184 E(Thermal)= 0.069905
E(SCF)= -265.732672 DE(MP2)= -0.930576
DE(CBS)= -0.091597 DE(MP34)= -0.031117
DE(CCSD)= -0.025389 DE(Int)= 0.029616
DE(Empirical)= -0.044321
CBS-QB3 (0 K)= -266.761873 CBS-QB3 Energy= -266.756152
CBS-QB3 Enthalpy= -266.755208 CBS-QB3 Free Energy= -266.791107

Oxetan-3-one

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.446557	-1.057599	0.000067
2	6	0	0.662738	-0.000023	-0.000031
3	8	0	1.854164	-0.000015	-0.000042
4	6	0	-0.446504	1.057607	0.000069
5	1	0	-0.492159	-1.685287	-0.896511
6	1	0	-0.492185	-1.684903	0.896924
7	1	0	-0.492061	1.685276	-0.896526
8	8	0	-1.435357	0.000024	-0.000137
9	1	0	-0.492113	1.684928	0.896913

Frequencies -- 155.4622 411.5422 451.7966
Frequencies -- 690.5075 766.7440 844.2960
Frequencies -- 997.5351 1000.4255 1070.1544
Frequencies -- 1079.9603 1119.8117 1155.6027
Frequencies -- 1271.6314 1315.1417 1463.7458
Frequencies -- 1492.8570 1910.6808 3014.1207
Frequencies -- 3026.6654 3067.9117 3068.9599

Rotational constants (GHZ): 12.16805 4.94675 3.68314

Zero-point correction= 0.066922 (Hartree/Particle)
Thermal correction to Energy= 0.071428
Thermal correction to Enthalpy= 0.072372

Thermal correction to Gibbs Free Energy= 0.039546

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.066253 E(Thermal)= 0.070786
E(SCF)= -265.695233 DE(MP2)= -0.933961
DE(CBS)= -0.091817 DE(MP34)= -0.031868
DE(CCSD)= -0.025291 DE(Int)= 0.029353
DE(Empirical)= -0.044446
CBS-QB3 (0 K)= -266.727009 CBS-QB3 Energy= -266.722476
CBS-QB3 Enthalpy= -266.721532 CBS-QB3 Free Energy= -266.754402

$CH_2OHCOCH_2O$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.524462	-1.173475	-0.248365
2	6	0	-0.735818	-0.344399	0.015498
3	8	0	-1.854928	-0.742362	-0.030439
4	6	0	-0.438546	1.217267	0.353533
5	1	0	0.350892	-2.177490	0.143323
6	1	0	0.587334	-1.242912	-1.347280
7	1	0	-0.096114	1.082672	1.402883
8	8	0	0.506888	1.667922	-0.459197
9	1	0	-1.408027	1.731007	0.312532
10	8	0	1.681459	-0.654442	0.337944
11	1	0	1.797967	0.241423	-0.021920

Frequencies -- 90.7136 152.3740 243.8744
Frequencies -- 296.5411 437.8443 510.7112
Frequencies -- 519.0911 588.2592 674.8615
Frequencies -- 854.7330 933.1614 992.7549
Frequencies -- 1108.9663 1140.9858 1213.6640
Frequencies -- 1231.3713 1273.2669 1345.4820
Frequencies -- 1445.4609 1467.7794 1483.0145
Frequencies -- 1856.7176 2850.8804 2959.1381
Frequencies -- 3015.8981 3099.8933 3648.4171

Rotational constants (GHZ): 4.31598 3.76537 2.20865

Zero-point correction= 0.080729 (Hartree/Particle)
Thermal correction to Energy= 0.087129
Thermal correction to Enthalpy= 0.088073

Thermal correction to Gibbs Free Energy= 0.049873

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.079922 E(Thermal)= 0.086362
E(SCF)= -341.149370 DE(MP2)= -1.140164
DE(CBS)= -0.117219 DE(MP34)= -0.045841
DE(CCSD)= -0.035382 DE(Int)= 0.036140
DE(Empirical)= -0.055420
CBS-QB3 (0 K)= -342.427334 CBS-QB3 Energy= -342.420893
CBS-QB3 Enthalpy= -342.419949 CBS-QB3 Free Energy= -342.458225

CH_2OOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.138777	0.267972	0.095284
2	8	0	0.077724	-0.560221	-0.084653
3	8	0	-1.147439	0.226518	-0.070254
4	1	0	-1.421096	0.106998	0.851602
5	1	0	1.086899	1.252009	-0.355730
6	1	0	2.059259	-0.297218	0.171687

Frequencies -- 158.4332 238.0112 479.7809
Frequencies -- 653.6144 840.9608 1134.1141
Frequencies -- 1191.7143 1362.9490 1431.5847
Frequencies -- 3114.7993 3259.4237 3742.9027

Rotational constants (GHZ): 53.22066 11.15021 9.61324
Zero-point correction= 0.040115 (Hartree/Particle)
Thermal correction to Energy= 0.044573
Thermal correction to Enthalpy= 0.045518
Thermal correction to Gibbs Free Energy= 0.014074

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.039713 E(Thermal)= 0.044190
E(SCF)= -189.239652 DE(MP2)= -0.624298
DE(CBS)= -0.064257 DE(MP34)= -0.024631
DE(CCSD)= -0.016314 DE(Int)= 0.019286
DE(Empirical)= -0.029984
CBS-QB3 (0 K)= -189.940136 CBS-QB3 Energy= -189.935660
CBS-QB3 Enthalpy= -189.934715 CBS-QB3 Free Energy= -189.966193

CH_2=C=O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.741834	0.938203	0.000123
2	6	0	1.206905	0.000001	-0.000030
3	1	0	1.741940	-0.938134	0.000123
4	6	0	-0.102453	-0.000017	-0.000042
5	8	0	-1.263811	0.000004	0.000023

Frequencies -- 447.6311 563.0714 596.0764
Frequencies -- 991.2716 1171.5786 1408.4117
Frequencies -- 2233.4304 3178.5376 3271.3229

ROTATIONAL CONSTANTS (GHZ) 284.86579 10.31697 9.95638

Zero-point correction= 0.031578 (Hartree/Particle)
Thermal correction to Energy= 0.035085
Thermal correction to Enthalpy= 0.036029
Thermal correction to Gibbs Free Energy= 0.007993

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.031263 E(Thermal)= 0.034782
E(SCF)= -151.781440 DE(MP2)= -0.534392
DE(CBS)= -0.052001 DE(MP34)= -0.016167
DE(CCSD)= -0.015375 DE(Int)= 0.017230
DE(Empirical)= -0.024911
CBS-Q (0 K)= -152.375794 CBS-Q Energy= -152.372274
CBS-Q Enthalpy= -152.371330 CBS-Q Free Energy= -152.399387

Cyclic Acetonyl peroxy r\radical

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.186927	1.158063	0.175274

2	6	0	0.449232	-0.202228	0.001204
3	6	0	-0.823489	-0.311496	0.933657
4	8	0	-1.579472	0.314241	-0.093863
5	8	0	-0.559202	-0.025822	-1.102578
6	8	0	1.261906	-1.181798	-0.080854
7	1	0	0.437816	1.946088	0.248231
8	1	0	1.813873	1.322730	-0.700136
9	1	0	1.805112	1.119087	1.071808
10	1	0	-0.828447	0.253435	1.866504
11	1	0	-1.090224	-1.360347	1.071142

Frequencies -- 189.6867 245.7548 287.4057
Frequencies -- 335.1460 413.2221 471.0073
Frequencies -- 561.9189 747.2802 793.5685
Frequencies -- 818.8773 888.1757 977.0889
Frequencies -- 1016.9654 1039.1632 1070.3348
Frequencies -- 1151.4436 1200.5475 1300.6461
Frequencies -- 1381.0758 1473.2553 1481.1875
Frequencies -- 1503.5092 3055.6587 3058.2869
Frequencies -- 3135.2664 3148.8694 3151.0123

Rotational constants (GHZ): 5.85680 3.51000 3.22190

Zero-point correction= 0.079500 (Hartree/Particle)
Thermal correction to Energy= 0.085453
Thermal correction to Enthalpy= 0.086397
Thermal correction to Gibbs Free Energy= 0.049838
Sum of electronic and zero-point Energies= -342.821514
Sum of electronic and thermal Energies= -342.815561
Sum of electronic and thermal Enthalpies= -342.814617
Sum of electronic and thermal Free Energies= -342.851176

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.078705 E(Thermal)= 0.084701
E(SCF)= -341.029279 DE(MP2)= -1.155328
DE(CBS)= -0.117324 DE(MP34)= -0.046984
DE(CCSD)= -0.037790 DE(Int)= 0.036014
DE(Empirical)= -0.054881
CBS-QB3 (0 K)= -342.326868 CBS-QB3 Energy= -342.320871
CBS-QB3 Enthalpy= -342.319927 CBS-QB3 Free Energy= -342.356561

TS0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.132329	1.362262	0.237229
2	6	0	-1.067168	-0.139034	0.042414
3	8	0	-1.736419	-0.721702	-0.801293
4	6	0	-0.140415	-0.882154	0.887962
5	1	0	-1.864510	1.788142	-0.446992
6	1	0	-1.400239	1.612602	1.268144
7	1	0	-0.148388	1.803807	0.043145
8	8	0	1.773480	-0.523273	-0.180477
9	1	0	0.277848	-0.448183	1.787749
10	1	0	-0.084976	-1.954556	0.754016
11	8	0	2.120406	0.638943	-0.319692

Frequencies -- -212.8703 38.5184 90.2399
Frequencies -- 120.1995 137.2177 282.8824
Frequencies -- 385.5468 521.8627 548.0691
Frequencies -- 624.2193 813.9585 832.1522
Frequencies -- 912.1359 1034.4812 1069.0655
Frequencies -- 1247.6137 1391.1747 1448.6327
Frequencies -- 1469.4341 1475.9303 1490.3987
Frequencies -- 1667.8389 3022.9765 3080.2547
Frequencies -- 3141.9983 3146.5387 3263.2727

Rotational constants (GHZ): 5.49342 2.16426 1.87594

Zero-point correction= 0.075764 (Hartree/Particle)
Thermal correction to Energy= 0.083186
Thermal correction to Enthalpy= 0.084130
Thermal correction to Gibbs Free Energy= 0.042500

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.075006 E(Thermal)= 0.082465
E(SCF)= -341.058350 DE(MP2)= -1.117252
DE(CBS)= -0.113420 DE(MP34)= -0.051993
DE(CCSD)= -0.040150 DE(Int)= 0.034191
DE(Empirical)= -0.061957
CBS-QB3 (0 K)= -342.333925 CBS-QB3 Energy= -342.326466
CBS-QB3 Enthalpy= -342.325522 CBS-QB3 Free Energy= -342.367236

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908027	1.132163	0.013837
2	6	0	-0.504591	-0.142725	0.028345
3	8	0	-0.620477	-1.315912	0.012164
4	1	0	-1.861343	1.341265	-0.458993
5	1	0	-0.296401	1.942660	0.367892
6	6	0	1.671614	0.146075	-0.031859
7	1	0	1.806831	0.067797	1.040788
8	1	0	1.876405	-0.739522	-0.618341
9	1	0	1.884345	1.102014	-0.490596

Frequencies -- -558.2245 50.1803 199.0673
Frequencies -- 310.7337 396.1399 480.2835
Frequencies -- 565.0295 608.4380 632.6400
Frequencies -- 897.4788 993.6879 1119.9937
Frequencies -- 1414.8308 1423.8855 1430.7847
Frequencies -- 2022.3587 3091.1217 3152.1034
Frequencies -- 3251.0652 3266.3612 3287.0081

Rotational constants (GHZ): 9.61305 7.34707 4.31289

Zero-point correction= 0.065140 (Hartree/Particle)
Thermal correction to Energy= 0.070943
Thermal correction to Enthalpy= 0.071887
Thermal correction to Gibbs Free Energy= 0.035977

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.064489 E(Thermal)= 0.070323
E(SCF)= -191.324964 DE(MP2)= -0.701882
DE(CBS)= -0.069933 DE(MP34)= -0.037665
DE(CCSD)= -0.023108 DE(Int)= 0.022889
DE(Empirical)= -0.033319
CBS-QB3 (0 K)= -192.103494 CBS-QB3 Energy= -192.097660
CBS-QB3 Enthalpy= -192.096716 CBS-QB3 Free Energy= -192.132688

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.170291	-1.101309	0.110765
2	6	0	0.944309	-0.043439	0.051268
3	6	0	0.498304	1.343171	0.331623
4	1	0	0.002858	-1.802687	0.929949
5	1	0	-0.184935	-1.638864	-0.842515
6	8	0	-1.433159	-0.491514	0.381002
7	8	0	-1.620567	0.512735	-0.586867
8	8	0	2.065788	-0.349483	-0.290306
9	1	0	1.135028	2.131281	-0.056559
10	1	0	0.042889	1.521026	1.304936
11	1	0	-0.726264	1.224790	-0.328378

Frequencies -- -1918.8551 110.0311 294.7692
Frequencies -- 397.4417 433.9617 488.3250
Frequencies -- 538.5391 573.4926 639.1432
Frequencies -- 791.9903 871.4845 916.2125
Frequencies -- 971.4750 1009.4560 1067.0155
Frequencies -- 1105.3578 1167.4497 1250.1681
Frequencies -- 1330.5285 1416.5617 1445.5392
Frequencies -- 1595.7350 1758.9834 3044.2778
Frequencies -- 3098.4500 3112.3182 3210.3058

Rotational constants (GHZ): 6.76778 2.91961 2.30061

Zero-point correction= 0.074357 (Hartree/Particle)
Thermal correction to Energy= 0.080048
Thermal correction to Enthalpy= 0.080992
Thermal correction to Gibbs Free Energy= 0.044521

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.073614 E(Thermal)= 0.079347
E(SCF)= -341.011058 DE(MP2)= -1.174017
DE(CBS)= -0.119886 DE(MP34)= -0.043626
DE(CCSD)= -0.037566 DE(Int)= 0.036353
DE(Empirical)= -0.055035
CBS-QB3 (0 K)= -342.331222 CBS-QB3 Energy= -342.325489
CBS-QB3 Enthalpy= -342.324545 CBS-QB3 Free Energy= -342.361087

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.388807	-0.752620	0.170707
2	6	0	0.977034	-0.142185	-0.014413
3	6	0	1.071257	1.361347	0.018408
4	8	0	1.916637	-0.889431	-0.172646
5	1	0	2.066488	1.668677	-0.298198
6	1	0	0.303754	1.806027	-0.619157
7	1	0	0.879219	1.717966	1.034464
8	8	0	-1.382199	0.035475	0.726159
9	8	0	-2.006479	0.157349	-0.631234
10	1	0	-0.421351	-1.811646	0.434528
11	1	0	-1.008688	-0.607426	-0.978080

Frequencies -- -1826.7608 92.3853 119.4485
Frequencies -- 131.3390 248.0364 457.1084
Frequencies -- 460.8091 531.9253 660.5935
Frequencies -- 783.0037 794.8105 840.4210
Frequencies -- 1001.9645 1048.2986 1083.5835
Frequencies -- 1111.4747 1232.1344 1307.8969
Frequencies -- 1393.4427 1462.1144 1467.5335
Frequencies -- 1766.6103 1958.9562 3043.5491
Frequencies -- 3102.4756 3103.2772 3152.1444

Rotational constants (GHZ): 6.92327 2.45570 2.08739

Zero-point correction= 0.073711 (Hartree/Particle)
Thermal correction to Energy= 0.080395
Thermal correction to Enthalpy= 0.081340
Thermal correction to Gibbs Free Energy= 0.042264

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.072974 E(Thermal)= 0.079697
E(SCF)= -340.993860 DE(MP2)= -1.154141
DE(CBS)= -0.118659 DE(MP34)= -0.051397
DE(CCSD)= -0.046258 DE(Int)= 0.036197
DE(Empirical)= -0.056457
CBS-QB3 (0 K)= -342.311602 CBS-QB3 Energy= -342.304879
CBS-QB3 Enthalpy= -342.303934 CBS-QB3 Free Energy= -342.343088

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.149873	-0.812680	0.191778
2	1	0	-0.402881	-1.123723	1.211625
3	1	0	-0.278331	-1.649079	-0.498004
4	6	0	1.193230	-0.127741	0.073684
5	6	0	0.809002	1.309299	0.123135
6	1	0	1.159773	1.983146	-0.651868
7	1	0	0.511383	1.750659	1.066247
8	8	0	-0.911596	0.341911	-0.200413
9	8	0	-2.518750	-0.197573	0.027840
10	1	0	-2.882842	0.369367	-0.667026
11	8	0	2.277689	-0.587293	-0.176496

Frequencies -- -799.8417 87.8924 118.0071
Frequencies -- 170.6578 240.3505 352.7048
Frequencies -- 434.2782 486.4276 580.4140
Frequencies -- 621.6977 815.6757 836.7771
Frequencies -- 894.1558 982.1031 1070.9442
Frequencies -- 1078.5971 1156.7340 1166.2705
Frequencies -- 1300.4567 1431.3539 1486.1372
Frequencies -- 1818.9840 3026.9762 3096.8899
Frequencies -- 3133.3173 3242.7326 3791.6718

Rotational constants (GHZ): 9.46007 2.11643 1.79821

Zero-point correction= 0.076141 (Hartree/Particle)
Thermal correction to Energy= 0.083086
Thermal correction to Enthalpy= 0.084030
Thermal correction to Gibbs Free Energy= 0.044637

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.075380 E(Thermal)= 0.082367
E(SCF)= -341.022753 DE(MP2)= -1.117735
DE(CBS)= -0.116414 DE(MP34)= -0.057462
DE(CCSD)= -0.053490 DE(Int)= 0.034626
DE(Empirical)= -0.057417
CBS-QB3 (0 K)= -342.315264 CBS-QB3 Energy= -342.308278
CBS-QB3 Enthalpy= -342.307333 CBS-QB3 Free Energy= -342.346811

TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.898642	1.346501	-0.374167
2	1	0	1.557771	2.169364	-0.122789
3	1	0	0.059865	1.510613	-1.031197
4	6	0	1.294840	0.113900	-0.031399
5	6	0	-0.461495	-1.059553	-0.299785
6	1	0	-0.221394	-1.616389	-1.199868
7	1	0	-0.387618	-1.532878	0.673161
8	8	0	2.054585	-0.676505	0.425072
9	8	0	-1.514286	-0.256231	-0.505934
10	8	0	-1.830834	0.433029	0.724956
11	1	0	-1.076265	1.061860	0.760046

Frequencies -- -267.6826 90.2443 155.0382
Frequencies -- 257.7691 311.7207 418.7942
Frequencies -- 437.6030 505.7998 510.6906
Frequencies -- 555.7609 669.6013 698.8446
Frequencies -- 869.6145 962.9366 1017.4049
Frequencies -- 1126.6298 1169.9918 1232.6915
Frequencies -- 1427.9457 1449.3902 1463.7649
Frequencies -- 1969.6582 3107.4518 3150.3867
Frequencies -- 3241.8420 3264.1699 3493.3243

Rotational constants (GHZ): 6.19718 2.34188 1.99040

Zero-point correction= 0.076453 (Hartree/Particle)
Thermal correction to Energy= 0.083195
Thermal correction to Enthalpy= 0.084139
Thermal correction to Gibbs Free Energy= 0.045376

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.075689 E(Thermal)= 0.082475
E(SCF)= -340.992885 DE(MP2)= -1.181352
DE(CBS)= -0.118913 DE(MP34)= -0.039001
DE(CCSD)= -0.036886 DE(Int)= 0.036458
DE(Empirical)= -0.053488
CBS-QB3 (0 K)= -342.310378 CBS-QB3 Energy= -342.303592
CBS-QB3 Enthalpy= -342.302647 CBS-QB3 Free Energy= -342.341495

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.394108	1.297655	0.457331
2	6	0	0.901218	-0.035090	0.085057
3	8	0	2.032712	-0.212412	-0.312461
4	6	0	-0.122546	-1.194061	0.099146
5	1	0	-0.192603	1.408941	1.360137
6	1	0	0.968788	2.150072	0.113379
7	1	0	0.091830	-1.861398	0.944933
8	8	0	-1.449366	-0.757566	0.237704
9	1	0	0.041010	-1.751291	-0.832629
10	8	0	-1.322743	0.772764	-0.592212
11	1	0	-2.030526	1.220358	-0.099282

Frequencies -- -1591.1075 109.3342 164.3114
Frequencies -- 322.7278 406.6314 473.4107
Frequencies -- 488.6139 532.1562 564.6658
Frequencies -- 649.4331 786.6128 866.6381
Frequencies -- 921.5209 947.8598 1008.1640
Frequencies -- 1083.1455 1178.9944 1216.5524
Frequencies -- 1332.9734 1435.4639 1463.9454
Frequencies -- 1747.1429 2991.5161 3033.3392
Frequencies -- 3139.0291 3251.8164 3747.8605

Rotational constants (GHZ): 5.89350 3.18228 2.33793

Zero-point correction= 0.077148 (Hartree/Particle)
Thermal correction to Energy= 0.083363
Thermal correction to Enthalpy= 0.084308
Thermal correction to Gibbs Free Energy= 0.046789

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.076376 E(Thermal)= 0.082636
E(SCF)= -341.012428 DE(MP2)= -1.103173
DE(CBS)= -0.114767 DE(MP34)= -0.060788
DE(CCSD)= -0.063354 DE(Int)= 0.034225
DE(Empirical)= -0.060115
CBS-QB3 (0 K)= -342.304023 CBS-QB3 Energy= -342.297763
CBS-QB3 Enthalpy= -342.296819 CBS-QB3 Free Energy= -342.334416

TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.125579	1.189688	0.258621
2	6	0	0.532544	-0.225079	0.018475
3	6	0	-0.807074	-0.462032	0.886604
4	8	0	-1.560356	0.294385	-0.023354
5	8	0	-0.646404	0.104964	-1.106701
6	8	0	1.327299	-1.140624	-0.200805
7	1	0	0.330092	1.912179	0.432895
8	1	0	1.703460	1.471078	-0.620556
9	1	0	1.787805	1.122513	1.123095
10	1	0	-0.858813	-0.064762	1.901236
11	1	0	-1.033153	-1.526273	0.828010

Frequencies -- -588.8650 238.6214 248.9243
Frequencies -- 298.3223 366.1365 421.1650
Frequencies -- 450.1550 624.6732 728.3396
Frequencies -- 802.0675 861.3066 995.0984
Frequencies -- 1015.1359 1027.0010 1064.4748
Frequencies -- 1193.6564 1254.3776 1358.7895
Frequencies -- 1447.8108 1474.7890 1476.5335
Frequencies -- 1499.8127 3054.5333 3064.5647
Frequencies -- 3141.7040 3145.4885 3156.7301

Rotational constants (GHZ): 5.76838 3.47153 3.15451

Zero-point correction= 0.078392 (Hartree/Particle)
Thermal correction to Energy= 0.084119
Thermal correction to Enthalpy= 0.085063
Thermal correction to Gibbs Free Energy= 0.048915
Sum of electronic and zero-point Energies= -342.821035
Sum of electronic and thermal Energies= -342.815308
Sum of electronic and thermal Enthalpies= -342.814364
Sum of electronic and thermal Free Energies= -342.850513

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.077608 E(Thermal)= 0.083377
E(SCF)= -341.010008 DE(MP2)= -1.160739
DE(CBS)= -0.118123 DE(MP34)= -0.046155
DE(CCSD)= -0.043479 DE(Int)= 0.036165
DE(Empirical)= -0.054856
CBS-QB3 (0 K)= -342.319586 CBS-QB3 Energy= -342.313818

CBS-QB3 Enthalpy= -342.312874 CBS-QB3 Free Energy= -342.349093

Table 1SI: Rate constants

T	k_3/s^{-1}			k_4/s^{-1}		
K	TST	CVT	CVT/SCT	TST	CVT	CVT/SCT
200	5.53E-18	2.42E-18	9.46E-12	2.64E-30	1.19E-30	8.86E-19
250	3.46E-12	1.78E-12	3.29E-08	7.76E-22	4.09E-22	6.02E-15
273	3.11E-10	1.69E-10	6.49E-07	5.59E-19	3.11E-19	1.99E-13
298	1.89E-08	1.07E-08	1.09E-05	2.27E-16	1.32E-16	6.52E-12
300	2.55E-08	1.45E-08	1.35E-05	3.52E-16	2.05E-16	8.51E-12
350	1.49E-05	9.16E-06	1.35E-03	3.92E-12	2.46E-12	3.53E-09
400	1.79E-03	1.17E-03	5.13E-02	4.32E-09	2.85E-09	5.34E-07
500	1.52E+00	1.07E+00	1.14E+01	8.02E-05	5.67E-05	1.26E-03
600	1.42E+02	1.05E+02	5.24E+02	5.75E-02	4.24E-02	3.38E-01
700	3.75E+03	2.86E+03	9.16E+03	6.38E+00	4.85E+00	2.18E+01
800	4.48E+04	3.50E+04	8.45E+04	2.20E+02	1.71E+02	5.36E+02
900	3.15E+05	2.51E+05	5.00E+05	3.48E+03	2.74E+03	6.74E+03
1000	1.52E+06	1.23E+06	2.14E+06	3.18E+04	2.53E+04	5.25E+04
1100	5.60E+06	4.58E+06	7.23E+06	1.95E+05	1.56E+05	2.86E+05
1200	1.68E+07	1.38E+07	2.03E+07	8.85E+05	7.14E+05	1.19E+06
1300	4.28E+07	3.56E+07	4.92E+07	3.19E+06	2.58E+06	3.99E+06
1400	9.62E+07	8.06E+07	1.06E+08	9.57E+06	7.79E+06	1.13E+07
1500	1.95E+08	1.65E+08	2.10E+08	2.48E+07	2.03E+07	2.81E+07
1600	3.65E+08	3.09E+08	3.82E+08	5.72E+07	4.69E+07	6.25E+07
1700	6.37E+08	5.42E+08	6.54E+08	1.19E+08	9.82E+07	1.27E+08
1800	1.05E+09	8.96E+08	1.06E+09	2.30E+08	1.90E+08	2.38E+08
1900	1.65E+09	1.41E+09	1.64E+09	4.13E+08	3.41E+08	4.19E+08
2000	2.48E+09	2.13E+09	2.43E+09	7.01E+08	5.80E+08	6.97E+08

Table 2SI: Rate constants

T	k_5/s^{-1}			k_6/s^{-1}			k_8/s^{-1}		
K	TST	CVT	SCT	TST	CVT	SCT	TST	CVT	SCT
250	8.80E-13	3.96E-13	3.01E-07	1.12E-15	9.27E-16	1.82E-15	1.86E-19	4.23E-20	1.41E-12
273	1.14E-10	5.37E-11	1.58E-06	2.40E-13	2.01E-13	3.47E-13	7.50E-17	1.92E-17	4.95E-11
298	9.72E-09	4.76E-09	8.93E-06	3.24E-11	2.73E-11	4.27E-11	1.79E-14	5.06E-15	1.54E-09
300	1.34E-08	6.59E-09	1.02E-05	4.62E-11	3.90E-11	6.06E-11	2.66E-14	7.60E-15	2.00E-09
350	1.33E-05	6.95E-06	3.56E-04	9.39E-08	7.99E-08	1.10E-07	1.29E-10	4.32E-11	6.05E-07
400	2.39E-03	1.30E-03	1.73E-02	2.89E-05	2.47E-05	3.13E-05	7.53E-08	2.85E-08	5.78E-05
500	3.50E+00	2.03E+00	1.05E+01	9.05E-02	7.78E-02	9.04E-02	5.70E-04	2.55E-04	4.84E-02
600	4.61E+02	2.78E+02	9.02E+02	1.98E+01	1.71E+01	1.90E+01	2.23E-01	1.11E-01	5.26E+00
700	1.53E+04	9.45E+03	2.30E+04	9.45E+02	8.16E+02	8.79E+02	1.60E+01	8.61E+00	1.66E+02
800	2.12E+05	1.34E+05	2.69E+05	1.73E+04	1.49E+04	1.58E+04	3.96E+02	2.26E+02	2.34E+03
900	1.66E+06	1.06E+06	1.86E+06	1.67E+05	1.44E+05	1.51E+05	4.84E+03	2.89E+03	1.91E+04
1000	8.60E+06	5.58E+06	8.83E+06	1.03E+06	8.86E+05	9.19E+05	3.60E+04	2.23E+04	1.05E+05
1100	3.32E+07	2.18E+07	3.19E+07	4.55E+06	3.93E+06	4.05E+06	1.86E+05	1.19E+05	4.36E+05
1200	1.03E+08	6.78E+07	9.38E+07	1.58E+07	1.37E+07	1.40E+07	7.37E+05	4.81E+05	1.45E+06
1300	2.68E+08	1.78E+08	2.35E+08	4.54E+07	3.93E+07	4.01E+07	2.36E+06	1.57E+06	4.05E+06
1400	6.09E+08	4.07E+08	5.19E+08	1.13E+08	9.73E+07	9.91E+07	6.44E+06	4.36E+06	9.89E+06
1500	1.25E+09	8.37E+08	1.03E+09	2.48E+08	2.14E+08	2.17E+08	1.54E+07	1.06E+07	2.16E+07
1600	2.33E+09	1.57E+09	1.90E+09	4.94E+08	4.27E+08	4.33E+08	3.30E+07	2.29E+07	4.31E+07
1700	4.06E+09	2.75E+09	3.25E+09	9.11E+08	7.88E+08	7.98E+08	6.48E+07	4.56E+07	7.98E+07
1800	6.65E+09	4.53E+09	5.25E+09	1.57E+09	1.36E+09	1.37E+09	1.18E+08	8.40E+07	1.39E+08
1900	1.04E+10	7.08E+09	8.08E+09	2.57E+09	2.22E+09	2.24E+09	2.03E+08	1.46E+08	2.28E+08
2000	1.55E+10	1.06E+10	1.19E+10	3.99E+09	3.45E+09	3.48E+09	3.31E+08	2.39E+08	3.59E+08