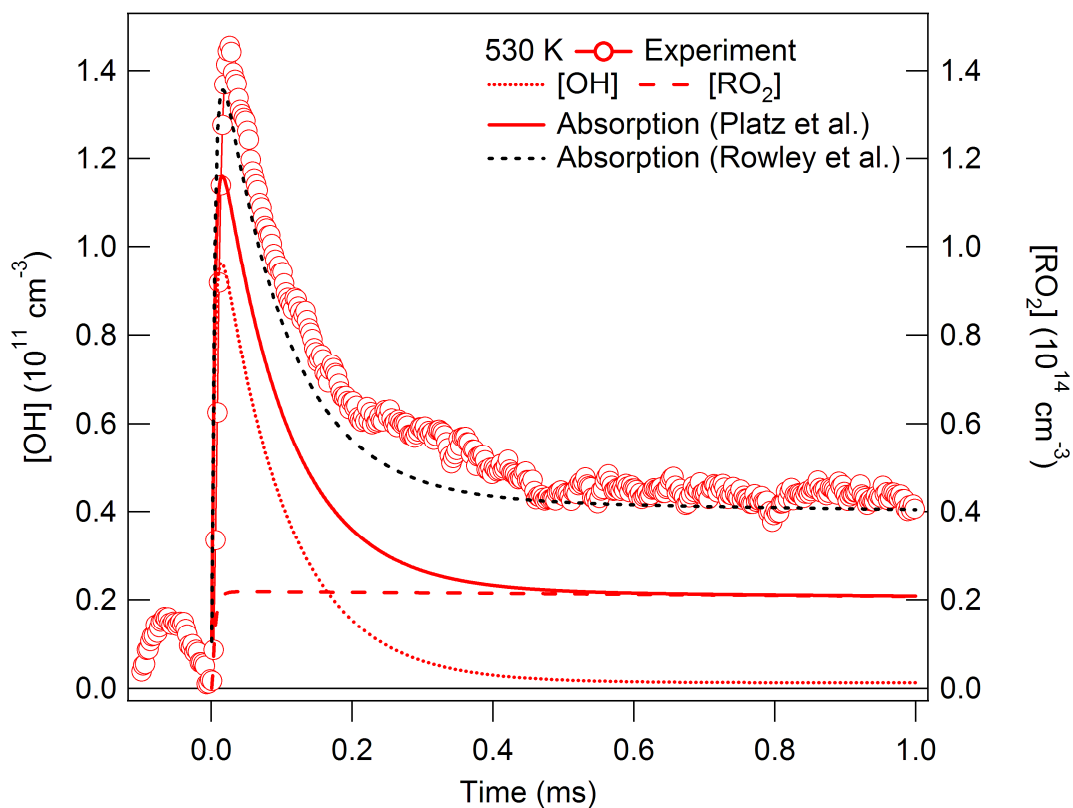
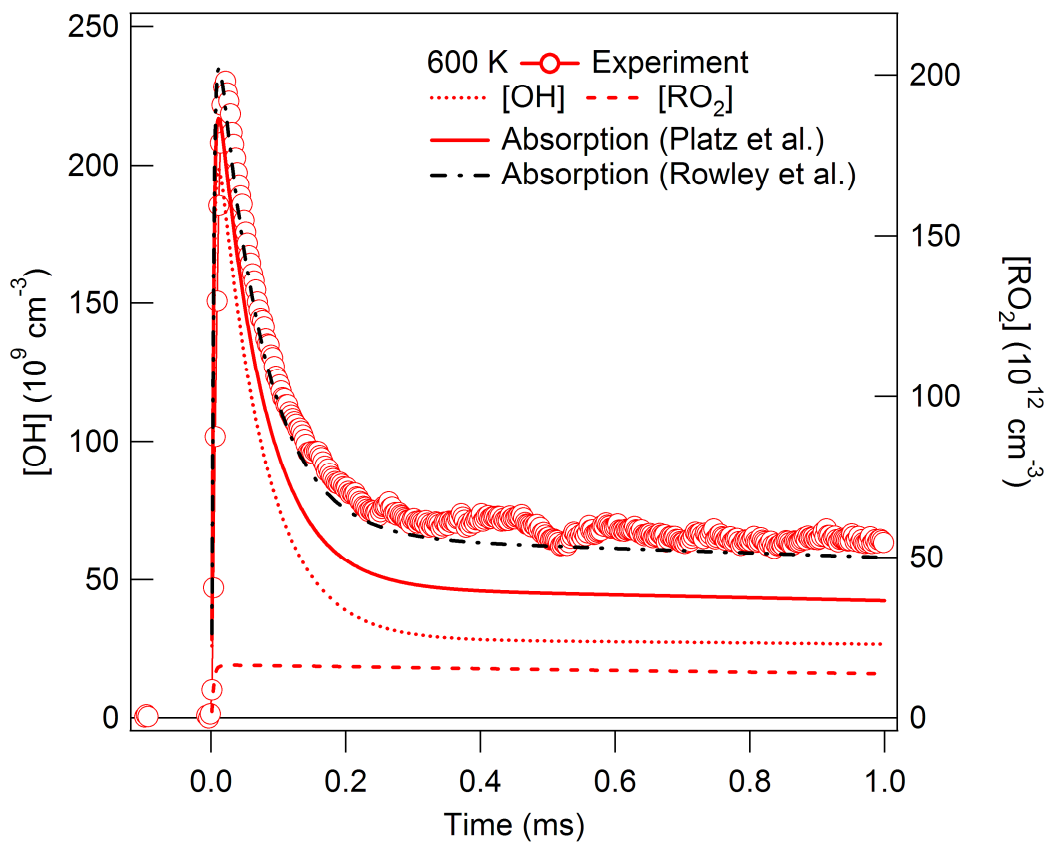
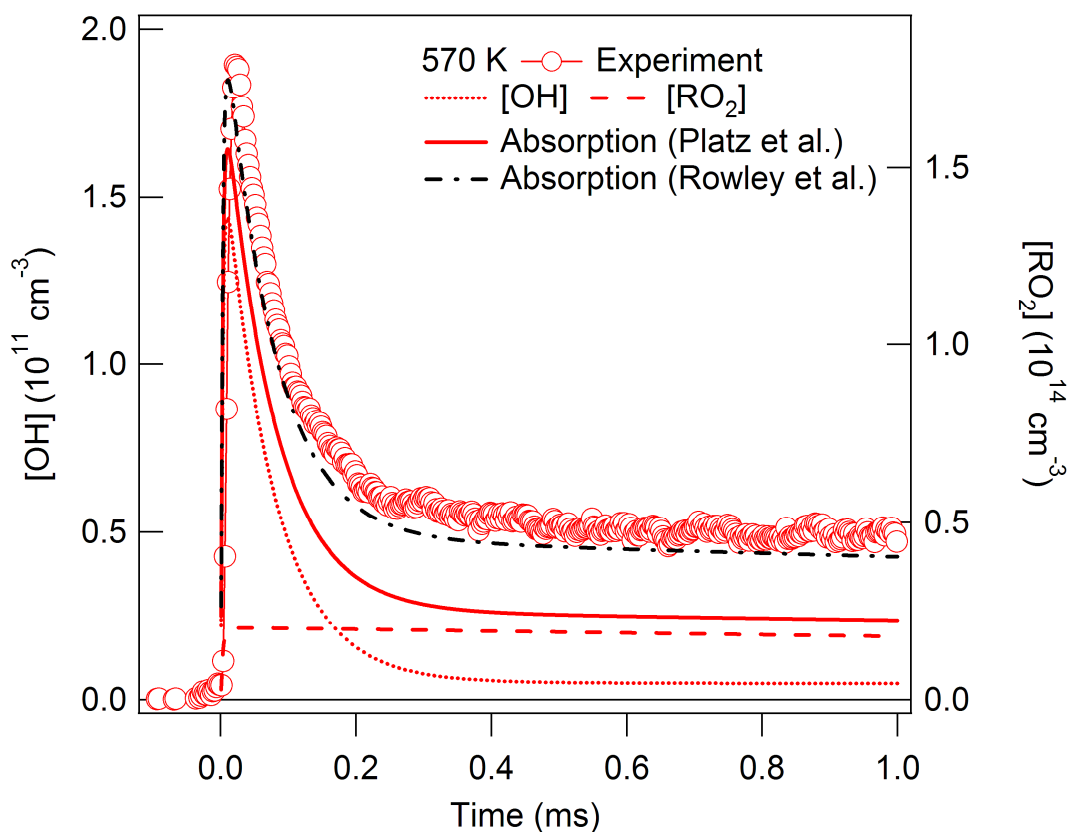
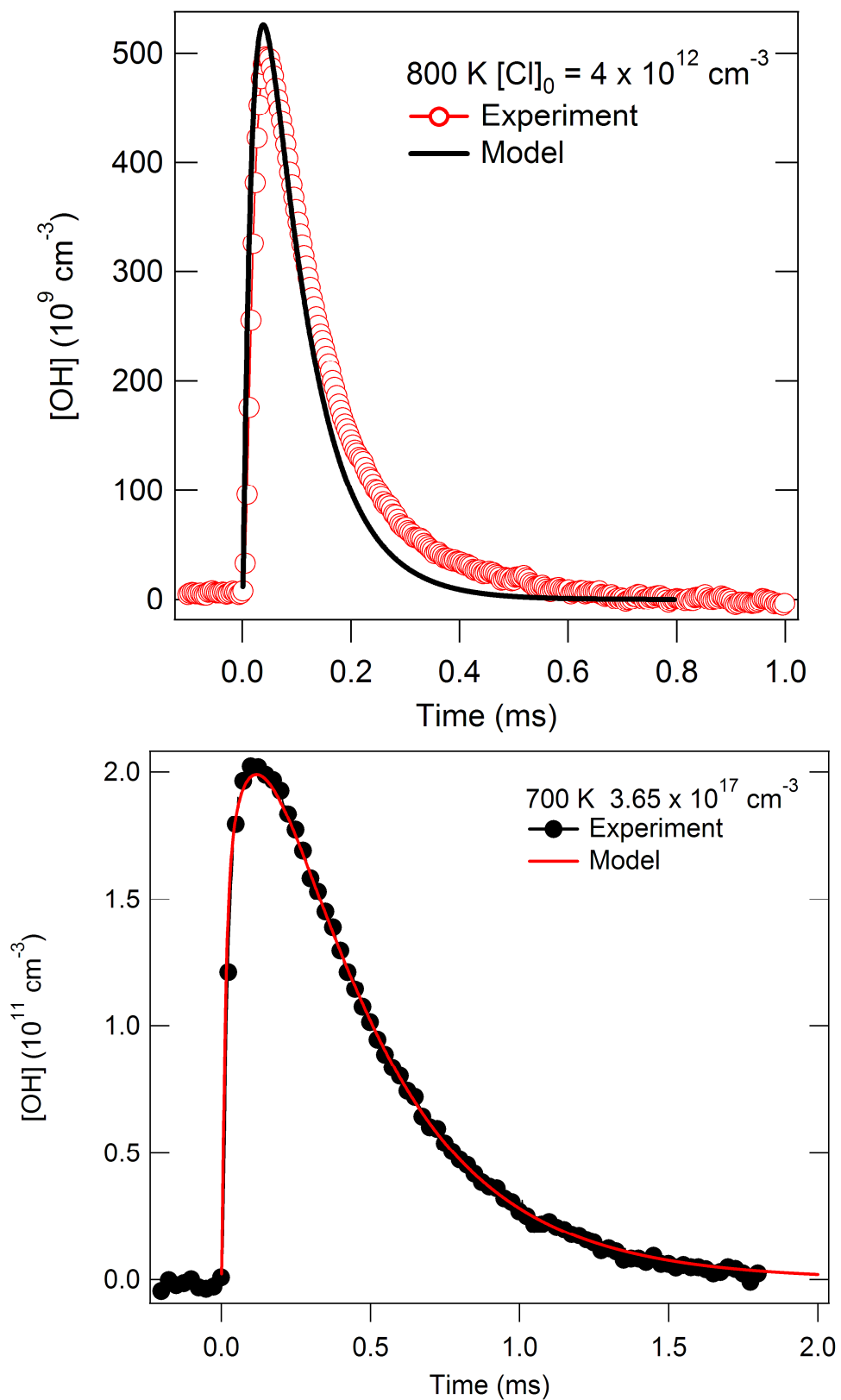


Supplementary Material for **Theory, Measurements, and Modeling of OH and HO<sub>2</sub> Formation in the Reaction of Cyclohexyl Radicals with O<sub>2</sub>** Adam M. Knepp, Giovanni Meloni, Leonard E. Jusinski, Craig A. Taatjes, Carlo Cavallotti, Stephen J. Klippenstein

Measured and Modeled OH profiles for 530 K, 570 K, 600 K, 800 K at total density of  $8.5 \times 10^{17} \text{ cm}^{-3}$  and for 700 K at total density of  $3.65 \times 10^{17} \text{ cm}^{-3}$ .





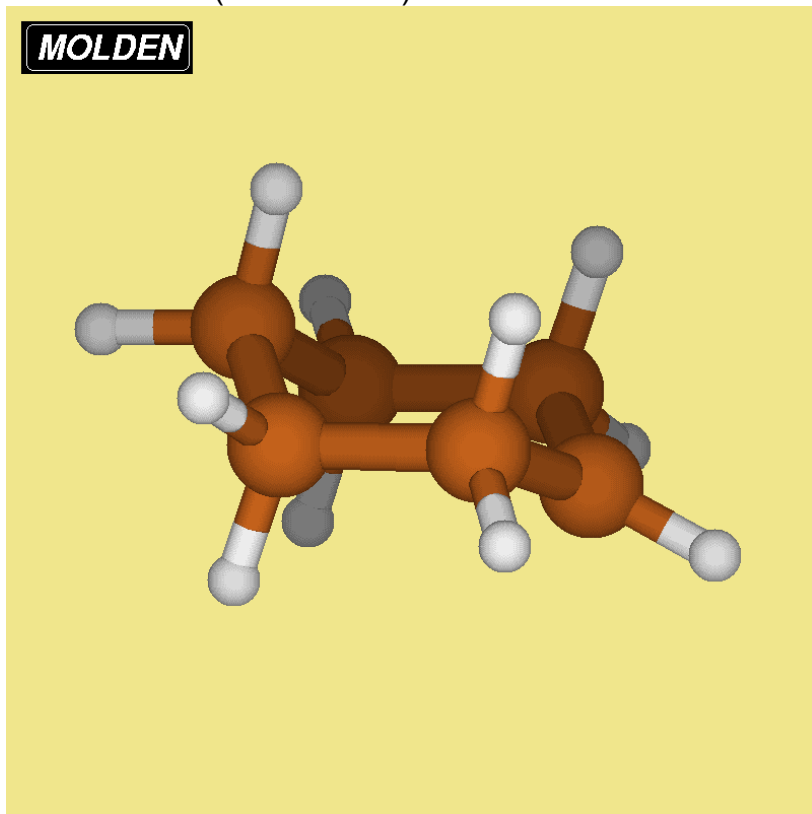


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b3lyp/6-311++G\*\*

cyclohexyl;chair

SCF Done: E(UB+HF-LYP) = -235.278935604 A.U. after 1 cycles



C	0.000000	-1.412877	0.264874
C	1.287463	0.778735	0.159028
C	-1.287463	0.778735	0.159028
C	-1.268558	-0.711882	-0.240862
C	1.268558	-0.711882	-0.240862
C	0.000000	1.463753	-0.166916
H	0.000000	-1.416881	1.363278
H	0.000000	-2.461864	-0.049357
H	1.471319	0.835683	1.248890
H	2.131986	1.291738	-0.311445
H	-1.471319	0.835683	1.248890
H	-2.131986	1.291738	-0.311445
H	-1.309650	-0.788778	-1.334059
H	-2.162096	-1.212434	0.146205
H	1.309650	-0.788778	-1.334059
H	2.162096	-1.212434	0.146205
H	0.000000	2.518836	-0.418841

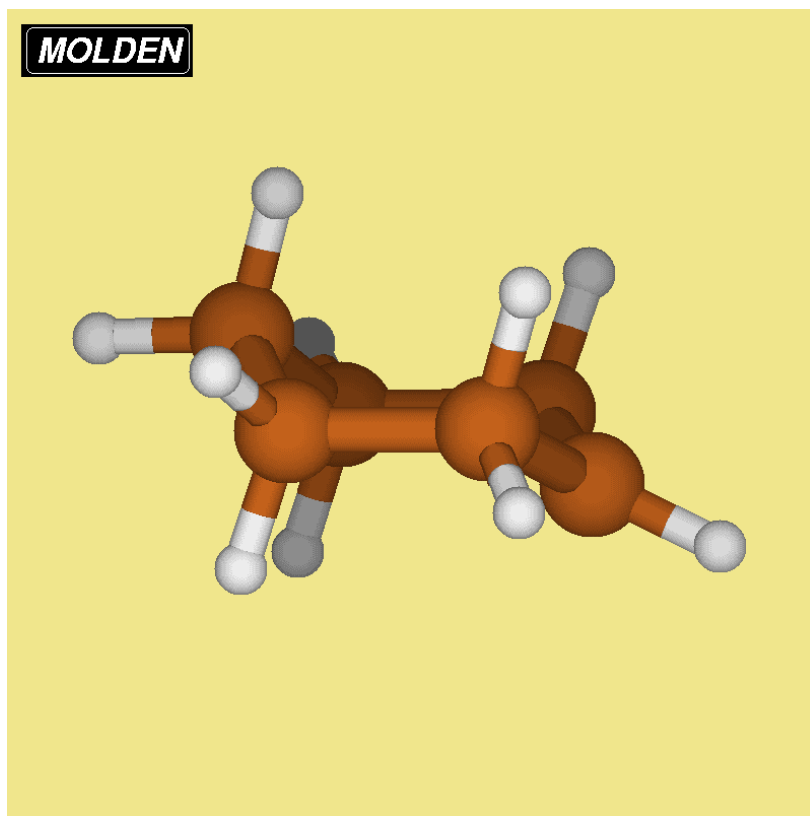
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Rotational constants (GHZ): 4.5091984 4.3193441 2.4689962  
Frequencies -- 174.6774 214.9902 327.4548

Frequencies --	391.6924	437.6793	458.3503
Frequencies --	607.3676	780.6128	804.8687
Frequencies --	852.4110	868.7978	875.2197
Frequencies --	924.0871	1012.8063	1029.8089
Frequencies --	1056.5062	1097.0436	1112.1687
Frequencies --	1128.4331	1152.6730	1252.7295
Frequencies --	1281.2878	1293.6761	1338.7834
Frequencies --	1345.0219	1350.6510	1376.1087
Frequencies --	1386.2957	1392.6464	1468.0436
Frequencies --	1471.5833	1487.6409	1491.2240
Frequencies --	1502.7902	2894.1520	2910.7902
Frequencies --	2995.4341	3009.4980	3010.1815
Frequencies --	3046.9340	3048.0661	3048.6941
Frequencies --	3050.1801	3061.6587	3160.5908

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cyC6H11 cyclo-Hexyl



C	1.290326	0.778229	0.155718
C	1.268024	-0.713120	-0.242113
H	2.134291	1.290108	-0.321850
H	1.483783	0.837360	1.244988
C	0.000017	-1.411394	0.270801
H	1.301642	-0.791881	-1.336922
H	2.164557	-1.215859	0.139694

H	0.000057	-2.465077	-0.033394
H	-0.000015	-1.404565	1.370711
C	-1.267971	-0.713152	-0.242183
C	-1.290360	0.778145	0.155783
H	-2.164527	-1.215979	0.139465
H	-1.301478	-0.791810	-1.337007
C	-0.000060	1.464702	-0.166024
H	-2.134406	1.290011	-0.321654
H	-0.000070	2.530092	-0.381002
H	-1.483694	0.837141	1.245074

Frequencies:

176.9268	214.9534	331.2502
387.4659	436.4939	458.4178
609.4810	784.3327	809.9209
856.0652	874.8035	878.3842
928.4547	1019.3797	1035.2139
1060.1512	1097.6133	1114.8457
1132.5924	1160.4875	1258.9795
1287.7283	1299.2161	1346.7490
1353.9826	1366.6427	1388.8981
1395.8779	1403.7213	1480.0708
1484.3525	1500.9188	1503.2790
1516.5526	2914.9040	2920.1861
3015.5172	3029.0034	3029.9272
3061.8407	3062.3787	3068.2578
3073.2496	3078.0208	3178.7043

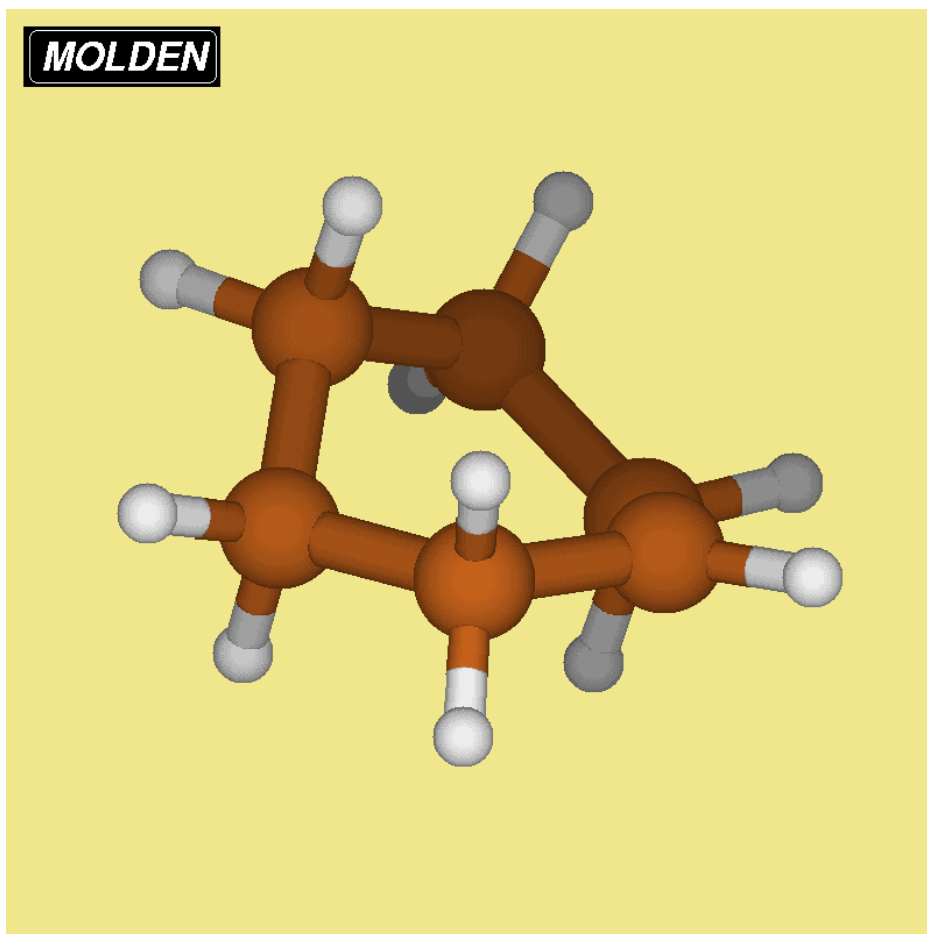
ROTATIONAL CONSTANTS (GHZ)      4.50574    4.31066    2.46557

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b3lyp/6-311++G\*\*

cyclohexyl;boat;a

SCF Done: E(UB+HF-LYP) = -235.272115843    A.U. after    1 cycles



C	-1.487283	0.362797	-0.113855
C	1.480842	-0.326147	-0.073667
C	0.951540	1.087586	0.306401
C	-0.943039	-0.974787	0.418967
C	0.346529	-1.349814	-0.323877
C	-0.395339	1.374492	-0.269419
H	0.895982	1.145083	1.408129
H	-0.739701	-0.894522	1.493684
H	0.120745	-1.392903	-1.395927
H	-0.625286	2.353715	-0.675063
H	-2.282880	0.740344	0.549435
H	2.136485	-0.682110	0.727588
H	2.102453	-0.250715	-0.970467
H	-1.983434	0.194970	-1.082489
H	1.673823	1.853550	0.012333
H	-1.696500	-1.759658	0.304761
H	0.678820	-2.352518	-0.039290

---

Rotational constants (GHZ): 4.5442982 4.2367669 2.5285700  
Frequencies -- 74.8731 182.2340 274.0188

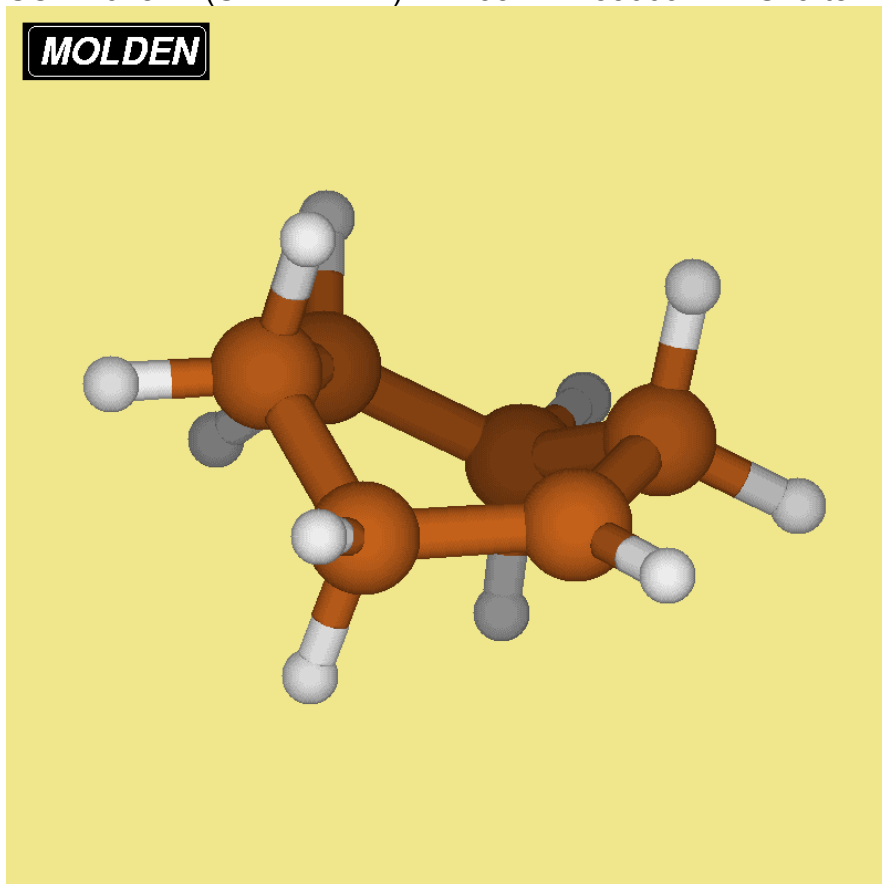
Frequencies --	372.7917	452.7628	478.0499
Frequencies --	611.8380	766.7110	801.0283
Frequencies --	837.8918	868.1521	878.1512
Frequencies --	923.1521	996.8391	1031.6324
Frequencies --	1055.7248	1087.3464	1124.5693
Frequencies --	1131.1953	1164.4068	1244.9589
Frequencies --	1260.4297	1292.8402	1320.9786
Frequencies --	1340.8361	1356.7523	1372.9267
Frequencies --	1377.0765	1393.7215	1465.2861
Frequencies --	1473.6191	1492.4306	1498.3909
Frequencies --	1510.9004	2906.5456	2941.1544
Frequencies --	2960.2601	3008.0374	3016.5115
Frequencies --	3024.0460	3047.9900	3058.0281
Frequencies --	3060.2798	3069.9539	3165.3250

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b3lyp/6-311++G\*\*

cyclohexyl;boat;b

SCF Done: E(UB+HF-LYP) = -235.272185663 A.U. after 1 cycles



C	0.167080	1.486413	-0.021200
C	-0.161835	-1.477900	-0.024402
C	-1.316343	-0.494965	-0.345686



C	1.325046	0.589743	-0.329798
C	1.154521	-0.769377	0.371318
C	-1.145517	0.870225	0.347743
H	-1.354409	-0.318846	-1.425893
H	1.416032	0.425837	-1.419024
H	1.163268	-0.594040	1.452664
H	-1.219984	0.729319	1.441216
H	0.277658	2.564011	-0.068019
H	0.011180	-2.116389	-0.896718
H	-0.457504	-2.149583	0.787830
H	-2.277052	-0.941411	-0.072662
H	2.269636	1.059244	-0.030959
H	2.007683	-1.420127	0.157986
H	-1.974215	1.537145	0.085734

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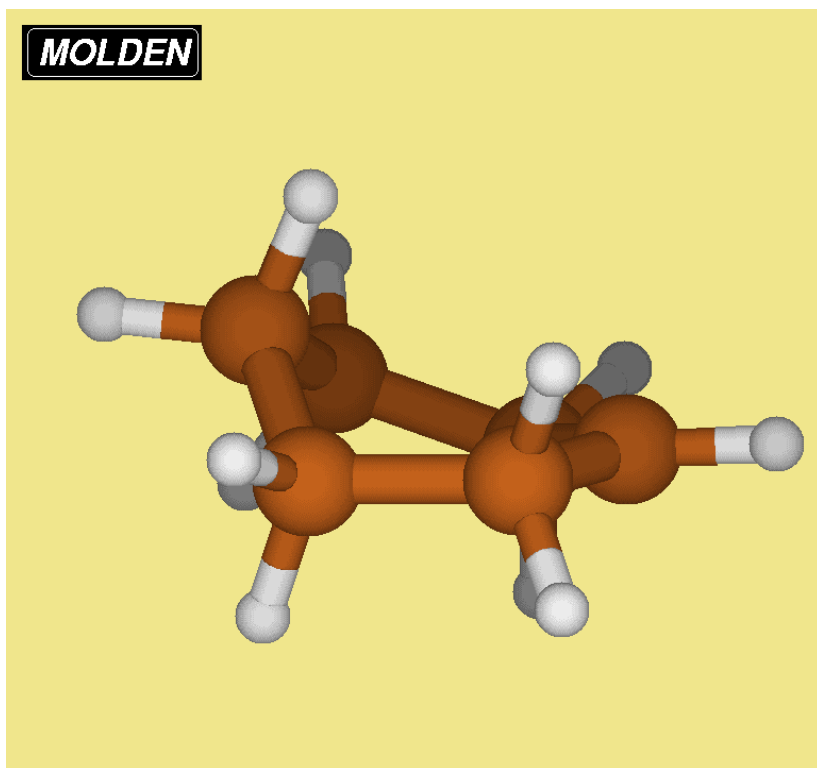
Rotational constants (GHZ):	4.3968866	4.3781173	2.5382607
Frequencies --	68.5175	223.5247	238.5114
Frequencies --	336.0618	455.7232	479.5517
Frequencies --	576.0133	767.3186	801.9733
Frequencies --	835.4703	873.4826	879.3935
Frequencies --	947.1907	1008.7731	1026.5353
Frequencies --	1052.1953	1078.9954	1125.1569
Frequencies --	1127.8358	1162.4681	1217.9831
Frequencies --	1276.1176	1291.1208	1336.0315
Frequencies --	1348.7987	1358.8130	1364.8937
Frequencies --	1382.3267	1388.1346	1469.4071
Frequencies --	1471.7095	1489.3579	1500.2376
Frequencies --	1513.2537	2906.7600	2909.3595
Frequencies --	3012.7011	3015.5505	3022.8386
Frequencies --	3027.8418	3035.1482	3042.2734
Frequencies --	3058.5442	3069.9316	3168.8103

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b3lyp/6-311++G\*\*

cyC6H11;chair <-> twist-boat; 2

SCF Done: E(UB+HF-LYP) = -235.271692976 A.U. after 1 cycles



C	-1.445805	0.532581	-0.052831
C	1.411849	-0.531728	0.056383
C	1.127774	0.997523	0.183298
C	-1.067724	-0.897458	0.369456
C	0.187400	-1.351119	-0.383618
C	-0.249986	1.415069	-0.222333
H	1.311528	1.301190	1.229237
H	-0.870643	-0.931294	1.448414
H	0.018962	-1.228113	-1.460884
H	-0.407386	2.442860	-0.534688
H	-2.155537	0.968100	0.669110
H	1.755659	-0.913027	1.023509
H	2.234802	-0.697068	-0.644941
H	-2.003999	0.491864	-1.001869
H	1.860989	1.567458	-0.397524
H	-1.905885	-1.575682	0.184433
H	0.380464	-2.415493	-0.216933

---

Rotational constants (GHZ):	4.5311614	4.2226058	2.4801633
Frequencies --	-118.5801	119.7232	281.6889
Frequencies --	412.6488	454.0372	474.9114
Frequencies --	651.2861	755.5324	790.2280
Frequencies --	843.3568	871.5876	873.0735
Frequencies --	912.3506	992.2301	1047.6647
Frequencies --	1054.3269	1082.5935	1127.3591

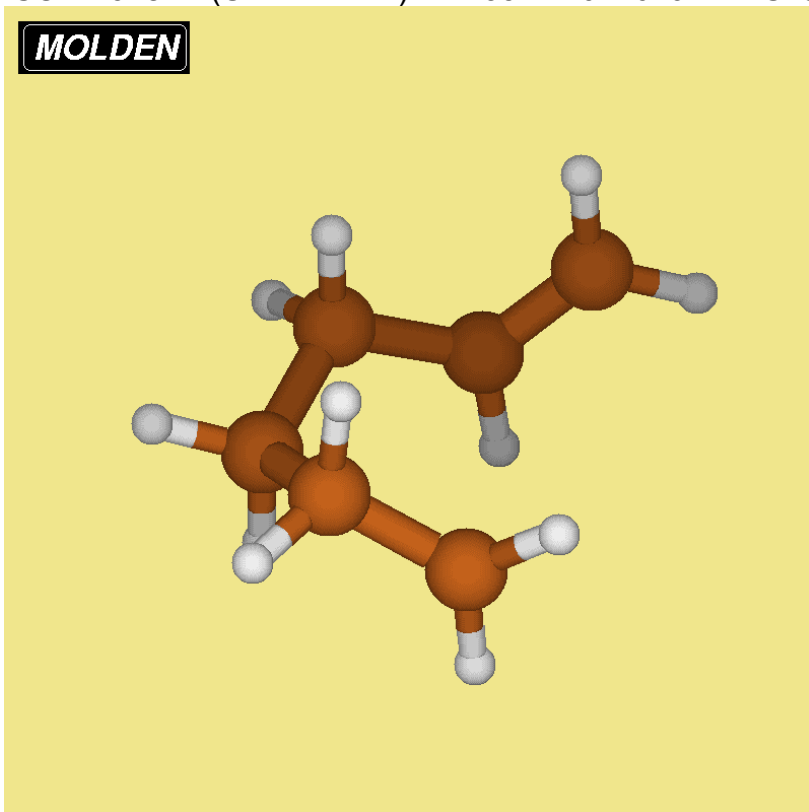
Frequencies --	1148.8912	1168.7885	1236.6772
Frequencies --	1263.1499	1293.8903	1328.2755
Frequencies --	1345.0633	1359.9845	1376.1105
Frequencies --	1379.0550	1401.7468	1466.9709
Frequencies --	1470.0335	1491.8917	1494.6953
Frequencies --	1507.4664	2903.2398	2944.3729
Frequencies --	2950.2086	3002.7834	3011.8348
Frequencies --	3020.2630	3025.0373	3051.5303
Frequencies --	3057.6341	3063.8633	3151.7491

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b3lyp/6-311++G\*\*

5-hexen-1-yl; from cyclohexyl chair

SCF Done: E(UB+HF-LYP) = -235.244077619 A.U. after 1 cycles



C	-1.682072	0.132269	-0.425899
C	2.262720	0.692974	-0.271709
C	0.554895	-1.152801	-0.105128
C	-0.948422	-1.067426	0.219028
C	-1.388086	1.451540	0.199979
C	1.390862	-0.026240	0.433877
H	-1.453644	0.160979	-1.496889
H	-2.762346	-0.074022	-0.353077
H	2.410893	0.525006	-1.334597
H	0.694254	-1.225528	-1.189919
H	2.855755	1.476895	0.185822

H	0.931624	-2.093801	0.318620
H	-1.088091	-1.031640	1.306407
H	-1.551692	1.598577	1.262109
H	-1.424611	-1.993560	-0.121380
H	-1.031073	2.294914	-0.375571
H	1.279550	0.180285	1.497584

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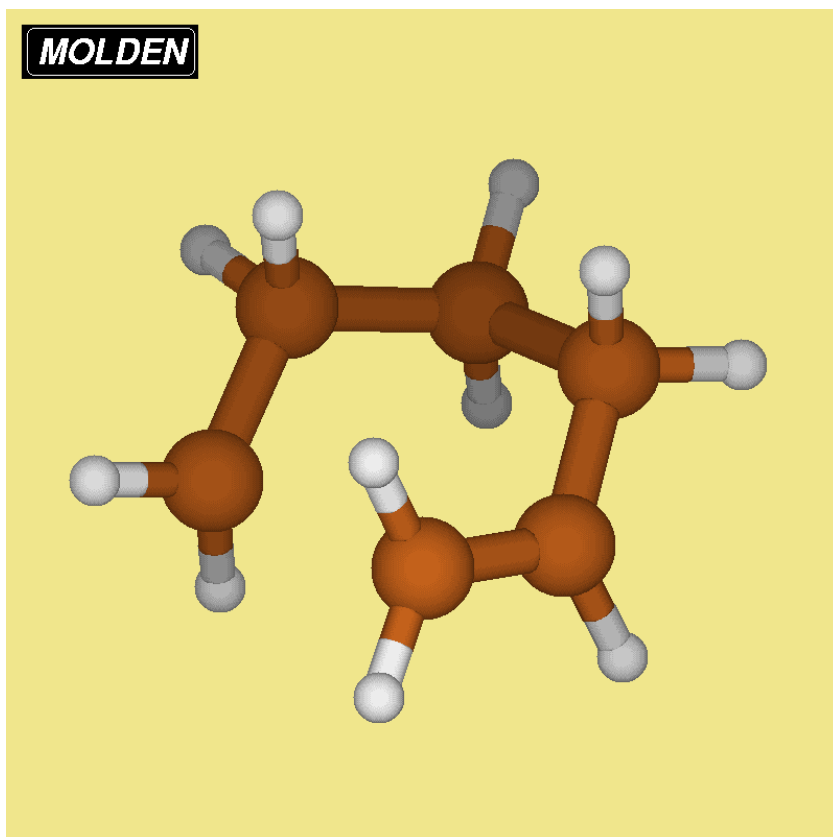
Rotational constants (GHZ):	5.0401662	2.4312003	1.8568460
Frequencies --	69.8598	84.4748	97.4533
Frequencies --	140.1232	282.7117	313.9780
Frequencies --	398.1832	454.5400	517.8709
Frequencies --	624.7869	785.8266	797.3115
Frequencies --	889.2795	924.4167	934.2400
Frequencies --	947.1861	1017.8623	1023.0827
Frequencies --	1054.9061	1090.0760	1177.0361
Frequencies --	1207.9208	1244.0041	1279.5103
Frequencies --	1321.3535	1349.6084	1361.1393
Frequencies --	1376.3533	1451.9315	1460.8852
Frequencies --	1474.8047	1478.3977	1491.3468
Frequencies --	1693.1412	2943.5075	2992.6753
Frequencies --	3010.3031	3035.3900	3037.4236
Frequencies --	3053.6860	3115.8782	3125.1467
Frequencies --	3134.5439	3207.1358	3240.5373

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b3lyp/6-311++G\*\*

cyC6H11;chair <-> 5-hexen-1-yl

SCF Done: E(UB+HF-LYP) = -235.229969366 A.U. after 1 cycles



C	1.485587	0.030410	0.269370
C	-1.255157	1.166736	0.276854
C	-0.749321	-1.266247	0.220743
C	0.731881	-1.216252	-0.235193
C	0.992774	1.340766	-0.278130
C	-1.482450	-0.054650	-0.275728
H	1.450804	0.051551	1.366713
H	2.551699	-0.093983	0.016886
H	-0.908683	1.254833	1.301189
H	-0.775383	-1.304654	1.316724
H	-1.681815	2.065962	-0.153533
H	-1.210695	-2.188797	-0.144273
H	0.773883	-1.246474	-1.330798
H	0.902994	1.438705	-1.355938
H	1.245186	-2.115440	0.122415
H	1.277699	2.251677	0.240706
H	-1.965569	-0.117953	-1.247583

---

Rotational constants (GHZ):	4.3490983	3.7368380	2.2932099
Frequencies --	-438.2568	160.8452	245.2759
Frequencies --	324.2855	367.5222	423.6909
Frequencies --	467.8799	534.0601	676.6183
Frequencies --	740.7097	805.9557	821.3554

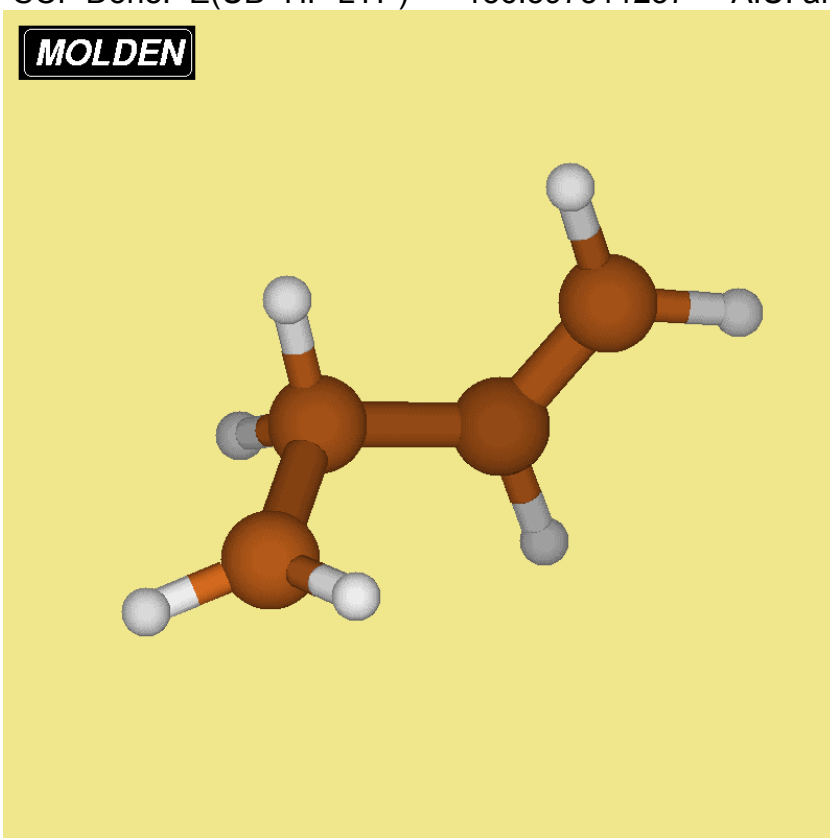
Frequencies --	880.7279	920.2055	928.8061
Frequencies --	943.3712	963.4661	1008.1239
Frequencies --	1027.9345	1079.0246	1156.1383
Frequencies --	1203.9811	1234.9583	1267.8282
Frequencies --	1289.6990	1334.1770	1360.5626
Frequencies --	1372.9274	1431.2151	1457.7776
Frequencies --	1471.3272	1486.9486	1494.2289
Frequencies --	1577.3384	2937.8534	3001.7314
Frequencies --	3007.3249	3014.0510	3049.8114
Frequencies --	3059.1549	3104.0737	3123.9668
Frequencies --	3137.3537	3194.0499	3207.6376

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b3lyp/6-311++G\*\*

c4h7

SCF Done: E(UB+HF-LYP) = -156.597511237 A.U. after 1 cycles



C	-1.797295	-0.047403	-0.266208
C	0.619097	0.549007	0.131529
C	1.757243	-0.352235	-0.222272
C	-0.663905	-0.189922	0.417036
H	-1.875137	0.641607	-1.102297
H	0.436465	1.271591	-0.681730
H	-2.687979	-0.611725	-0.013683
H	0.894162	1.153915	1.005624

H	1.588209	-1.239018	-0.821312
H	2.779126	-0.077033	0.008343
H	-0.625689	-0.896016	1.244544

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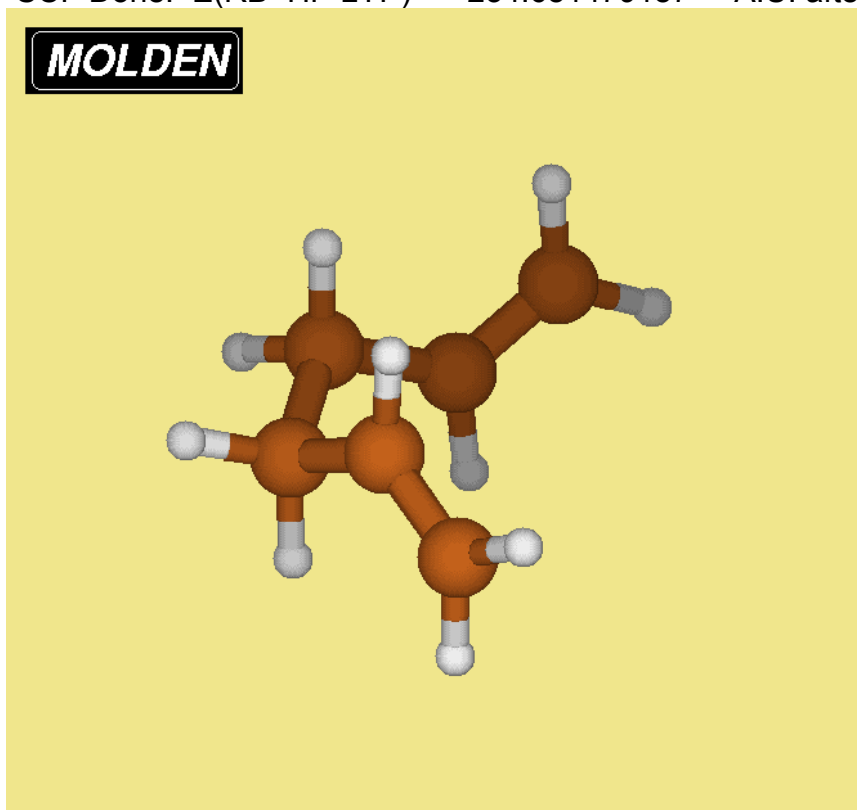
Rotational constants (GHZ):	24.8059123	4.3248066	4.2107596
Frequencies --	97.8826	127.9030	325.9391
Frequencies --	420.0317	501.7130	657.7403
Frequencies --	797.8602	895.8261	946.2540
Frequencies --	1024.7109	1044.7598	1075.5725
Frequencies --	1111.7344	1238.1891	1318.6168
Frequencies --	1335.7668	1443.3382	1457.2641
Frequencies --	1461.2298	1695.7710	2937.6748
Frequencies --	3009.6335	3121.2917	3129.4909
Frequencies --	3135.4422	3208.3970	3240.7000

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b3lyp/6-311++G\*\*

C6H10;hexadiene

SCF Done: E(RB+HF-LYP) = -234.681479187 A.U. after 1 cycles



C

1.507682	-0.095200	-0.462638	
C	-2.257016	-0.976984	-0.194630
C	-0.757304	1.048353	-0.159194
C	0.757302	1.048352	0.159192
C	2.257019	-0.976981	0.194631
C	-1.507684	-0.095198	0.462639

H	1.416498	-0.186378	-1.544715
H	-2.375061	-0.931737	-1.273387
H	-0.906975	1.043945	-1.244458
H	-2.779505	-1.775334	0.320402
H	-1.177002	1.992470	0.211039
H	0.906974	1.043946	1.244456
H	2.375068	-0.931730	1.273387
H	1.177001	1.992468	-0.211042
H	2.779509	-1.775331	-0.320399
H	-1.416504	-0.186372	1.544716

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Rotational constants (GHZ):	5.8757844	2.0698219	1.7195566
Frequencies --	58.5004	95.6928	101.6788
Frequencies --	265.1234	340.8482	421.3098
Frequencies --	436.6839	620.2658	660.1703
Frequencies --	824.0955	871.8644	940.4488
Frequencies --	941.5051	944.8160	983.7642
Frequencies --	1023.2883	1024.1754	1032.1611
Frequencies --	1052.4989	1190.3280	1237.6349
Frequencies --	1247.7993	1322.8280	1323.1902
Frequencies --	1345.6730	1361.3440	1448.6317
Frequencies --	1454.1891	1477.3000	1486.3444
Frequencies --	1701.2738	1701.6919	2998.7994
Frequencies --	3009.6222	3039.1426	3053.7520
Frequencies --	3110.8838	3112.3113	3125.0995
Frequencies --	3125.4535	3207.1484	3207.3404

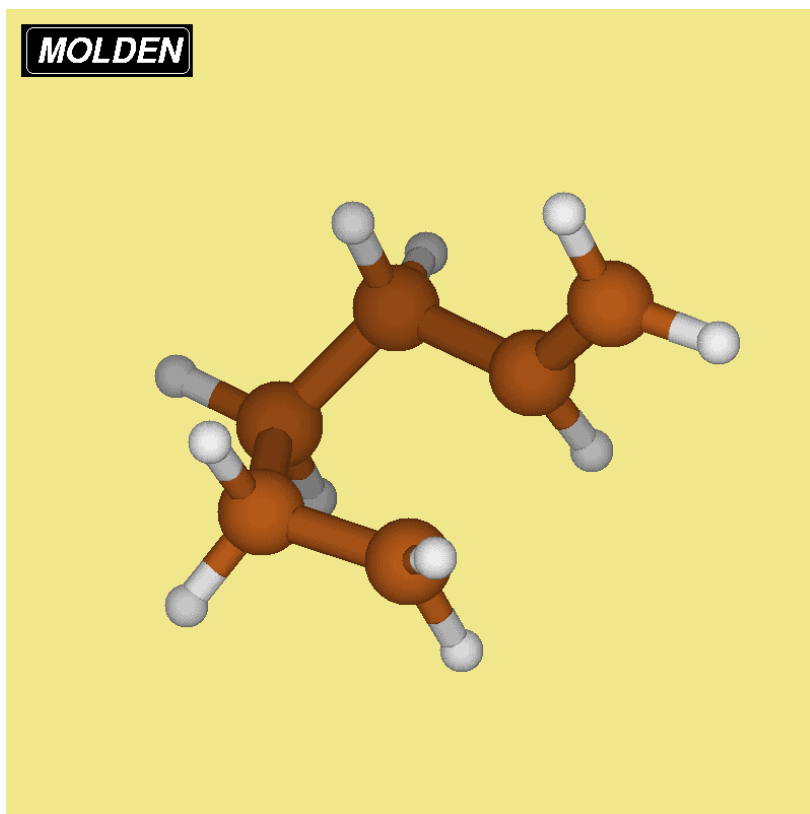
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b3lyp/6-311++G\*\*

5-hexen-1-yl <-> c5h9ch2

SCF Done: E(UB+HF-LYP) = -235.233723239 A.U. after 1 cycles





C	-1.527192	0.552966	-0.378540
C	2.217823	0.222926	-0.270417
C	0.159160	-1.237925	-0.079448
C	-1.309525	-0.870728	0.163644
C	-0.474328	1.455128	0.191579
C	1.091115	-0.150749	0.413445
h	-1.459584	0.538650	-1.471706
h	-2.538749	0.903089	-0.128910
h	2.359508	-0.047371	-1.311965
h	0.329152	-1.398648	-1.150247
h	2.962761	0.871029	0.176183
h	0.404876	-2.180391	0.424063
h	-1.519650	-0.885491	1.240241
h	-0.564842	1.739642	1.236490
h	-1.987239	-1.592072	-0.303648
h	-0.010724	2.203983	-0.439970
h	1.082172	0.017864	1.487892

---

Rotational constants (GHZ):	5.3814876	2.9270921	2.1649939
Frequencies --	-461.0426	100.6326	247.4372
Frequencies --	281.3295	393.5287	414.7822
Frequencies --	513.4935	564.5527	578.7632
Frequencies --	784.4280	810.4113	826.5639
Frequencies --	848.0813	895.7186	921.1659

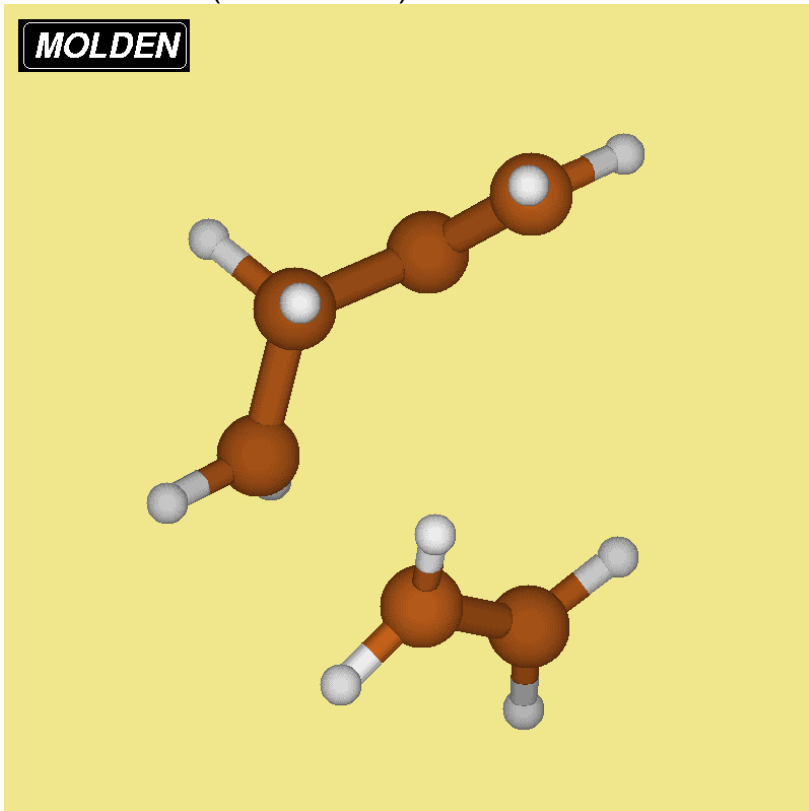
Frequencies --	923.0337	979.8945	1005.8075
Frequencies --	1024.8282	1070.4408	1177.3958
Frequencies --	1180.6940	1238.4017	1253.5656
Frequencies --	1278.5262	1335.4095	1344.7752
Frequencies --	1358.7284	1434.0821	1464.7659
Frequencies --	1479.5923	1483.7082	1498.7145
Frequencies --	1543.7176	2982.0133	3009.3120
Frequencies --	3013.1068	3039.6036	3046.5530
Frequencies --	3063.7090	3109.7110	3123.2256
Frequencies --	3127.4295	3205.8363	3215.6405

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b3lyp/6-311++G\*\*

5-hexen-1-yl <-> c4h7+c2h4

SCF Done: E(UB+HF-LYP) = -235.200574407 A.U. after 1 cycles



C	-1.876082	-0.123302	0.575561
C	2.061406	-1.173980	0.249603
C	0.964703	1.092703	0.160748
C	-0.428086	1.445242	-0.283550
C	-2.073259	-1.140072	-0.305768
C	1.507404	-0.177345	-0.436477
H	-1.191271	-0.246422	1.406546
H	-2.625287	0.651776	0.689229
H	2.149293	-1.141593	1.331781
H	1.021263	1.046038	1.254555

H	2.449307	-2.057589	-0.244808
H	1.638471	1.919416	-0.130741
H	-0.666325	1.321524	-1.335119
H	-2.856924	-1.095849	-1.054170
H	-0.885994	2.312480	0.184061
H	-1.406878	-1.993878	-0.341395
H	1.437833	-0.255382	-1.520637

---

Rotational constants (GHZ):	4.3536995	2.0835353	1.5930239
Frequencies --	-415.1211	43.0994	71.2947
Frequencies --	85.9991	185.2223	233.0437
Frequencies --	315.4192	385.5760	441.5984
Frequencies --	552.5244	644.2274	768.2531
Frequencies --	820.2422	851.3358	857.0873
Frequencies --	889.3522	942.1264	972.9240
Frequencies --	993.1769	1014.0136	1028.3570
Frequencies --	1063.4775	1175.6374	1226.2955
Frequencies --	1239.0007	1292.7437	1318.9751
Frequencies --	1340.2614	1449.9005	1457.6294
Frequencies --	1463.7008	1466.0314	1569.1832
Frequencies --	1700.1178	2913.7075	3027.2682
Frequencies --	3105.8454	3117.6162	3125.9774
Frequencies --	3126.8990	3135.5625	3198.5338
Frequencies --	3203.0277	3207.0403	3229.7502

\*\*\*\*\*

b3lyp/6-311++G\*\*

SCF Done: E(UB+HF-LYP) =	-235.272115843	A.U. after	1 cycles
Frequencies --	74.8731	182.2340	274.0188
Frequencies --	372.7917	452.7628	478.0499
Frequencies --	611.8380	766.7110	801.0283
Frequencies --	837.8918	868.1521	878.1512
Frequencies --	923.1521	996.8391	1031.6324
Frequencies --	1055.7248	1087.3464	1124.5693
Frequencies --	1131.1953	1164.4068	1244.9589
Frequencies --	1260.4297	1292.8402	1320.9786
Frequencies --	1340.8361	1356.7523	1372.9267
Frequencies --	1377.0765	1393.7215	1465.2861
Frequencies --	1473.6191	1492.4306	1498.3909
Frequencies --	1510.9004	2906.5456	2941.1544
Frequencies --	2960.2601	3008.0374	3016.5115
Frequencies --	3024.0460	3047.9900	3058.0281
Frequencies --	3060.2798	3069.9539	3165.3250

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b3lyp/6-311++G\*\*

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b3lyp/6-311++G\*\*

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b3lyp/6-311++G\*\*

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b3lyp/6-311++G\*\*

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b3lyp/6-311++G\*\*

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b3lyp/6-311++G\*

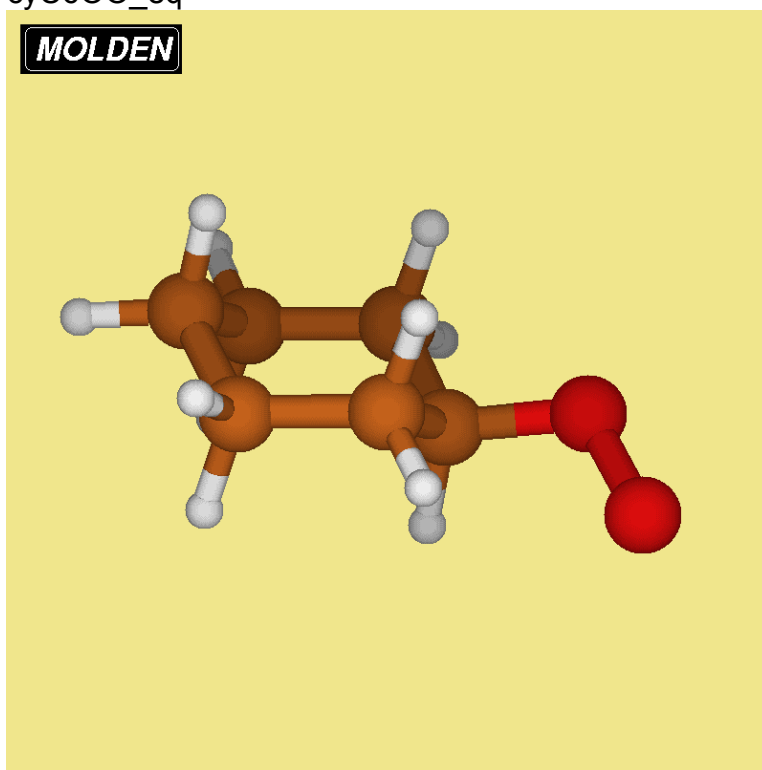
\*

Reactants and Products structures

all structures optimized at the b3lyp/6-31g(d,p) level  
and used as input for g2mp2 calculations

\*\*\*\*\*

cyC6OO\_eq



C	0.010095	-0.004451	0.029601
C	0.003404	-0.054601	1.555596
C	1.434176	0.080576	2.102054
C	2.367071	-0.981874	1.500272
C	2.342872	-0.943209	-0.035588
C	0.910647	-1.071033	-0.585047
H	-0.427157	-1.014780	1.869026
H	2.049965	-1.976872	1.842087
H	2.967145	-1.742291	-0.450159
H	0.900728	-0.985416	-1.676850

H	-0.648140	0.736686	1.938432
H	0.503305	-2.059131	-0.334596
H	2.780035	0.003588	-0.381775
H	3.390689	-0.837811	1.864439
H	1.420825	0.005630	3.194961
O	-1.342807	-0.250831	-0.487697
O	-2.143229	0.778619	-0.263320
H	0.288285	0.996383	-0.319858
H	1.821324	1.081074	1.863888

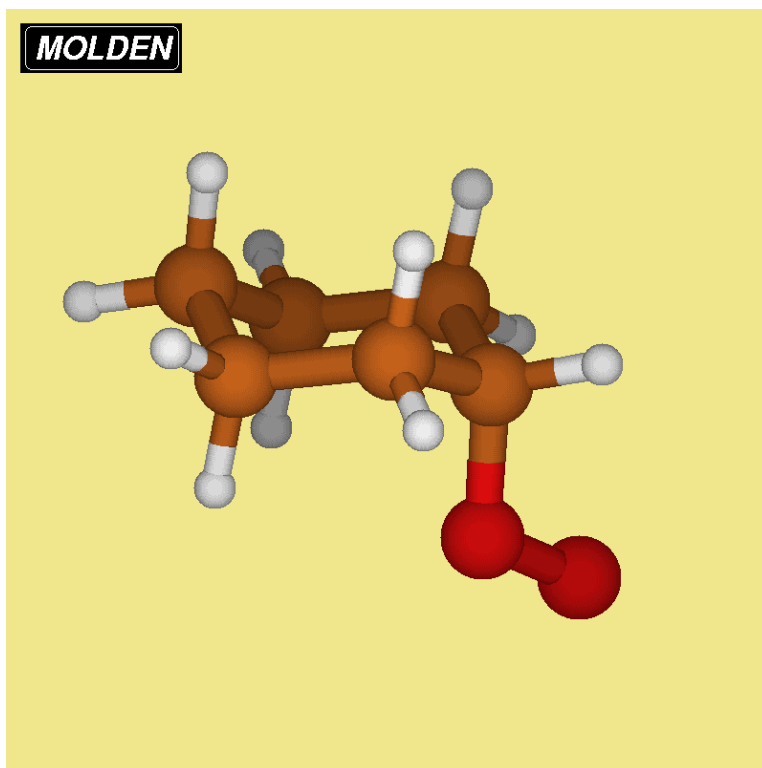
ROTATIONAL CONSTANTS (GHZ)            4.04077    1.38611    1.10989

Frequencies:

83.8871	134.6935	223.8552
250.7989	325.0532	366.2790
439.9799	457.6906	505.7405
566.6995	799.6513	808.6485
850.3549	897.7256	905.2842
926.0635	940.5576	1023.1363
1049.5417	1067.2527	1090.3593
1108.5818	1174.9947	1197.0793
1218.1058	1274.6323	1288.7369
1292.0283	1333.0805	1337.3389
1372.9293	1387.0258	1388.3946
1393.2463	1400.2086	1496.9965
1500.1917	1503.5305	1509.2144
1523.6405	3025.5773	3027.2799
3032.3268	3040.3592	3043.2163
3067.5581	3079.6222	3082.4653
3086.2899	3096.5461	3107.5816

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cyC6OO\_ax



```
C 0.0713164811 -0.3429513509 -0.9643894762
C -0.0141016178 1.1819250291 -1.00769392
C -0.034001064 1.8112879914 0.395567027
C -1.1271993838 1.1886024667 1.2768235631
C -0.9691611976 -0.3370320546 1.3621400933
C -0.9569732206 -0.9829673306 -0.0318648394
H -0.9366467937 1.4402837859 -1.5439245693
H -2.1149357257 1.4301289739 0.857983185
H -1.775308789 -0.7743482383 1.9617931531
H -0.7492277191 -2.0557576762 0.0274809146
H 0.8179657285 1.5752525812 -1.6019882701
H -1.9418046889 -0.8709883258 -0.5048326048
H -0.030348097 -0.5767701645 1.8769675517
H -1.0987073538 1.6284885141 2.2802984587
H -0.1792898271 2.8940047212 0.3094154648
H 0.9437159764 1.6622187117 0.8702576126
H 0.0102568732 -0.7766060709 -1.9674202577
O 1.4374487533 -0.6498917864 -0.4883037363
O 1.7169325509 -1.9362451284 -0.6053869295
Rotational constants (GHZ): 3.29941 1.64945 1.36980
```

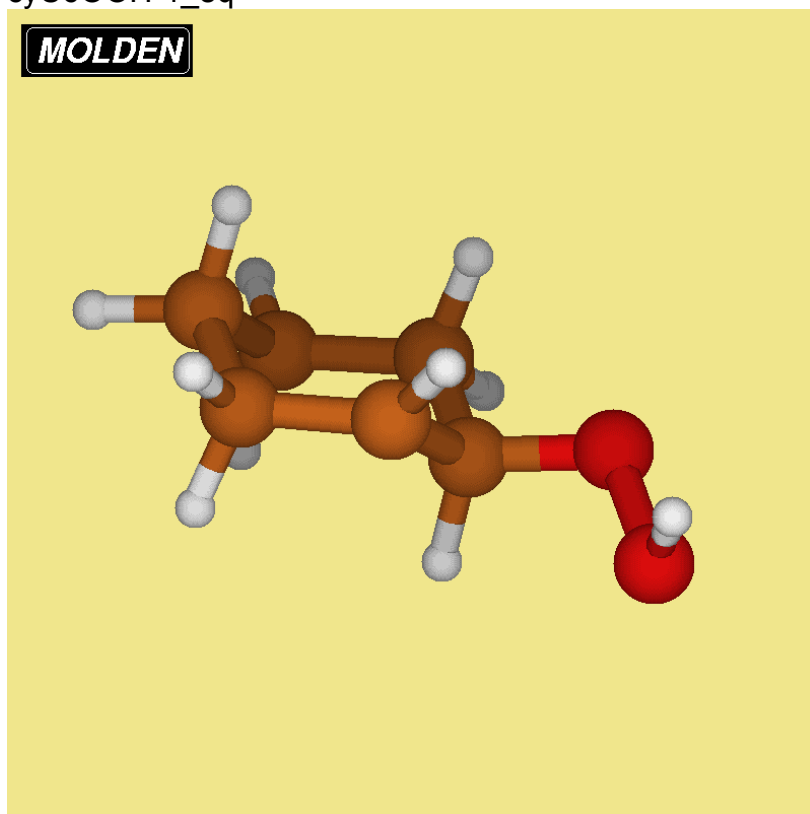
Frequencies:

83.5636	139.4992	185.8637
291.8822	319.4698	375.9297

424.8142	480.0362	541.3621
637.1707	783.5741	804.0497
819.1485	872.7898	876.2189
908.6041	944.0501	1037.2637
1040.1254	1050.3218	1091.7548
1138.8570	1148.9256	1175.2759
1213.5543	1268.6248	1296.1720
1303.8162	1346.1530	1353.7921
1366.2109	1390.5614	1394.9365
1400.0000	1402.3127	1485.4371
1492.3763	1501.7323	1504.8555
1519.4484	3018.4237	3037.3839
3041.4541	3043.8070	3044.0998
3076.2406	3083.1116	3084.3329
3088.0658	3093.3260	3103.5336

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cyC6OOH-1\_eq



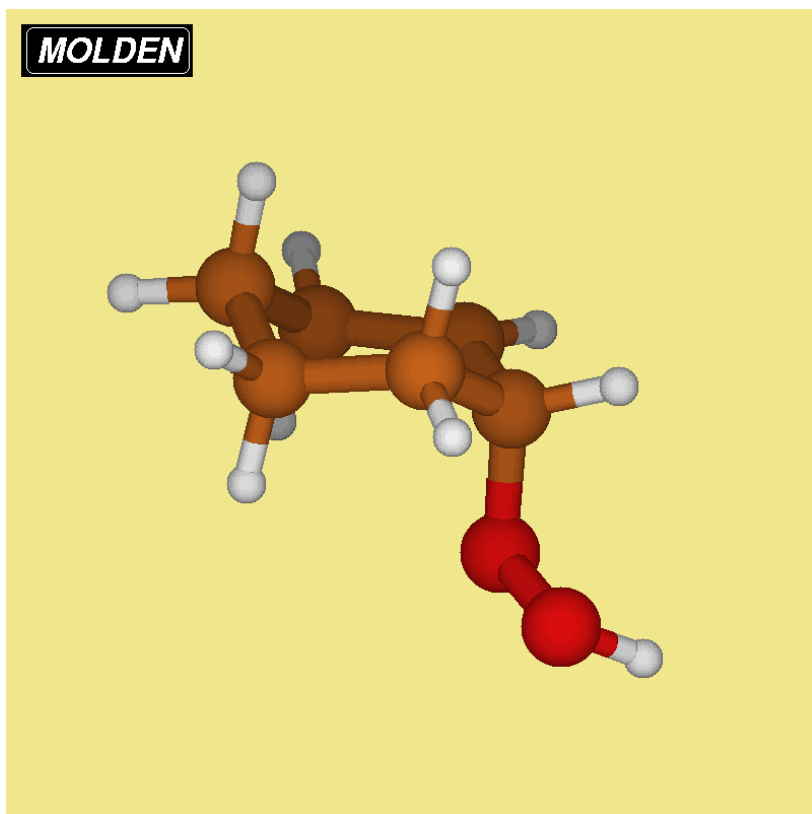
C	0.01088	-0.05568	-0.08674
C	0.01495	-0.09387	1.4088
C	1.34528	0.0391	2.08047
C	2.34953	-0.99341	1.50186
C	2.38572	-0.92842	-0.03291

C	0.99036	-1.10619	-0.65561		
H	-0.81848	-0.57335	1.91602		
H	2.04816	-2.00082	1.81684		
H	3.06186	-1.69559	-0.42725		
H	1.02898	-1.01333	-1.74624		
H	0.6	-2.10475	-0.42355		
H	2.80013	0.04034	-0.3455		
H	3.3498	-0.81554	1.91478		
H	1.2575	-0.07686	3.16541		
O	-1.26022	-0.36307	-0.66182		
O	-2.13647	0.77343	-0.41201		
H	0.32571	0.93845	-0.44576		
H	1.75732	1.04604	1.9031		
H	-2.69699	0.41262	0.29409		
ROTATIONAL CONSTANTS (GHZ)		4.06508	1.35255	1.08959	
Frequencies:					
83.8107	106.0644	149.7749			
199.5264	241.4566	303.1064			
345.4698	366.5663	451.7681			
490.5381	534.2612	583.3375			
802.0971	839.0711	871.3575			
905.8489	910.4549	942.1348			
974.8308	1027.5326	1061.1206			
1074.7318	1113.9392	1133.4425			
1143.5214	1200.1432	1258.8014			
1274.5671	1307.7429	1328.1650			
1341.8021	1352.6838	1360.0594			
1370.9671	1387.5941	1412.0770			
1491.8096	1498.3125	1502.3147			
1513.7014	2977.0246	2986.9351			
3025.9748	3033.1957	3045.1317			
3075.2377	3081.0627	3088.6635			
3097.3704	3181.4694	3756.6140			

\*\*\*\*\*

cyC6OOH-1\_ax





```
C 0.1886477359 1.2661334967 0.8259043744
C 0.6364127828 -0.1570865872 0.728012802
C -0.5201673055 -1.1279952068 0.4608835127
C -1.4438761249 -0.6236872136 -0.6555960058
C -2.0079001919 0.7636198626 -0.3190229736
C -0.8776495498 1.7860998992 -0.0835681286
O 1.5828508419 -0.1537229756 -0.3804675115
O 2.213541933 -1.4739241433 -0.4377386018
H -1.0907812881 -1.2397156521 1.3929916515
H -2.6227183589 0.6928833596 0.5884327117
H -1.2811754226 2.7304831296 0.3015141111
H 3.099667407 -1.246207807 -0.1119452905
H -0.1020553675 -2.1092008661 0.2180625128
H 0.8126390238 1.9658007842 1.3752043534
H -0.4228742304 2.0330878191 -1.0606308638
H -2.6664901714 1.1194025336 -1.1195316028
H -2.2608411592 -1.3367336863 -0.8152877056
H -0.8766373678 -0.5744996653 -1.5932571815
H 1.1873206566 -0.4566285043 1.6304147244
```

Frequencies:

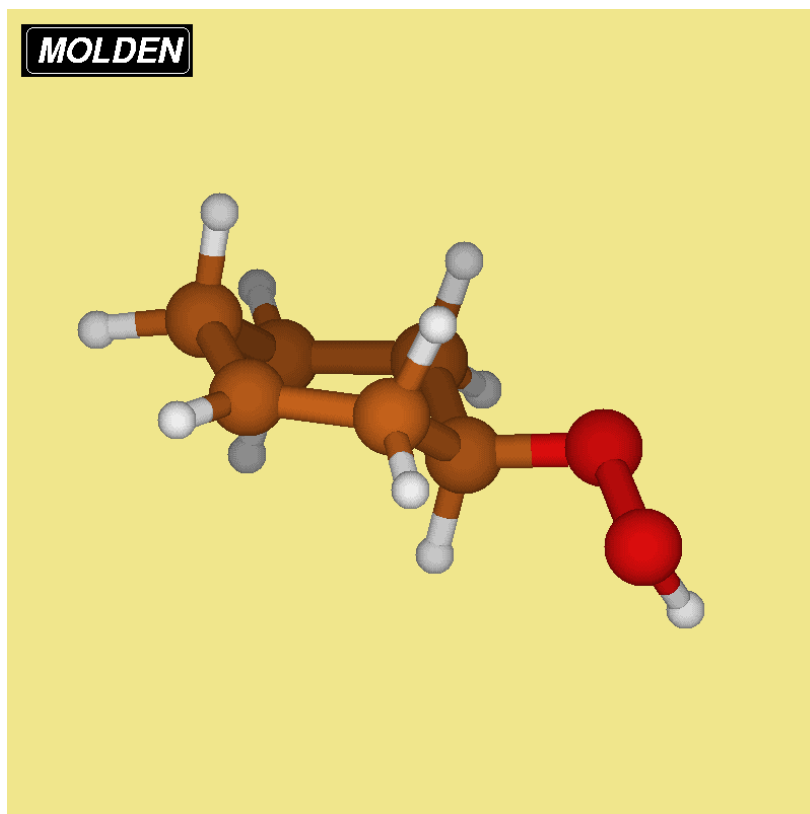
77.2568	135.7988	171.8288
230.9537	276.4140	291.7720

345.8429	419.6379	460.8119
520.1561	576.5942	669.7006
792.7425	813.8224	865.5291
875.1509	883.0163	909.8930
931.7463	1022.9129	1047.6676
1059.7889	1090.1600	1134.1560
1157.7871	1184.3105	1266.7137
1297.4654	1330.6480	1341.0062
1357.0571	1361.5818	1372.9215
1395.8744	1408.5868	1410.6110
1476.2601	1492.6318	1502.9928
1513.6829	2947.1412	3018.5077
3028.8235	3037.4030	3043.8971
3059.8089	3077.2169	3087.9118
3106.9414	3184.8447	3752.3424

Rotational constants (GHZ):      3.53184    1.54553    1.27750

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cyC6OOH-2\_eq



C	0.08945	0.30395	-0.13252
C	-0.03619	-0.14426	1.33373
C	1.20052	0.1778	2.112

C	2.53534	-0.13329	1.51198
C	2.60851	0.29336	0.03061
C	1.38958	-0.20296	-0.76315
H	-0.21413	-1.23591	1.31326
H	2.72549	-1.22283	1.56403
H	3.52888	-0.08588	-0.4275
H	1.44381	0.12777	-1.80598
H	-0.92629	0.30397	1.78374
H	1.36827	-1.30072	-0.77393
H	2.65398	1.38851	-0.02618
H	3.34249	0.33787	2.08448
H	1.12393	0.41532	3.16893
O	-0.95674	-0.22564	-0.95199
O	-2.21536	0.34537	-0.48783
H	-2.40895	0.94219	-1.22918
H	0.05954	1.40302	-0.18468

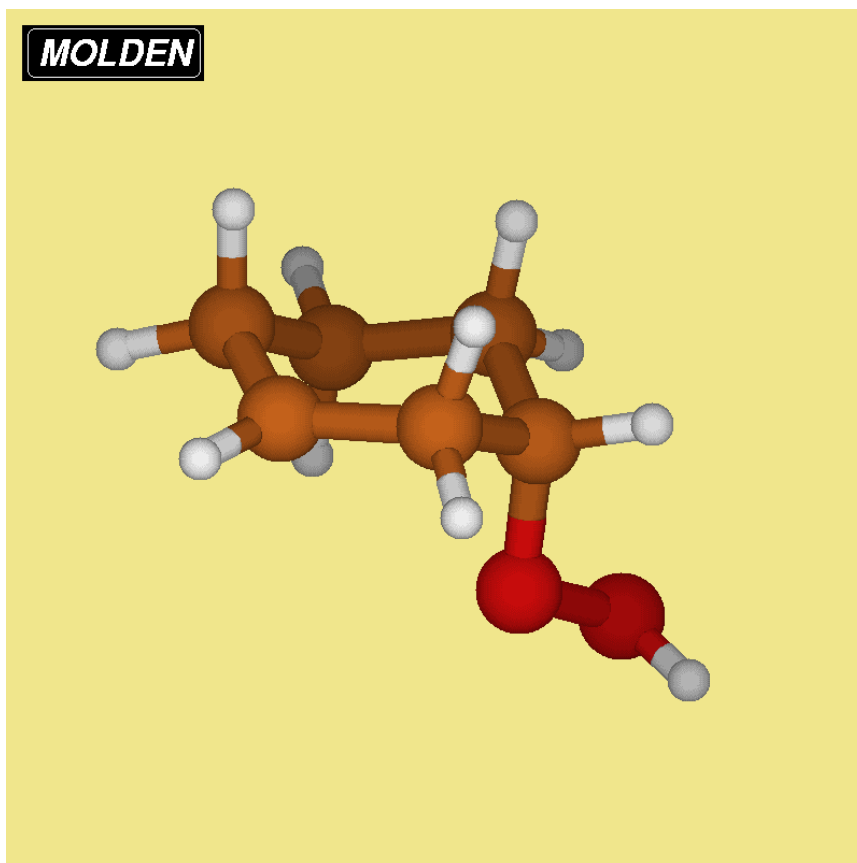
Frequencies:

103.1164	141.0394	175.5112
208.5540	235.9236	289.3816
363.0671	384.7608	460.4758
463.9463	507.5678	621.4435
797.5307	849.3771	865.2122
899.7235	923.7782	935.8344
962.4589	1042.5850	1052.8033
1091.6371	1101.5708	1118.9210
1139.1716	1227.8364	1249.5737
1281.1827	1310.1387	1333.3806
1357.3201	1360.0658	1369.6264
1393.1380	1394.2219	1406.9988
1481.1083	1485.6856	1505.2074
1514.8223	2925.7098	2941.6344
3004.9006	3036.3293	3039.9916
3069.8442	3082.6174	3092.1376
3103.8655	3189.4564	3752.6845

ROTATIONAL CONSTANTS (GHZ)      4.12575    1.35982    1.09116

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cyC6OOH-2\_ax



C	-0.063256	-0.992532	0.884123
C	-0.628235	0.410727	0.635002
C	0.487331	1.457633	0.454725
C	1.575996	0.998106	-0.462545
C	2.075777	-0.407403	-0.360687
C	0.917915	-1.416702	-0.216890
O	-1.381395	0.474998	-0.587111
O	-2.543404	-0.390797	-0.433989
H	0.887945	1.656371	1.467119
H	2.734696	-0.510004	0.524411
H	1.313104	-2.416145	-0.002357
H	-0.894319	-1.700123	0.956685
H	0.047484	2.401178	0.113187
H	0.440365	-0.987144	1.861275
H	0.374786	-1.479671	-1.165756
H	2.700293	-0.659999	-1.225391
H	2.133362	1.734915	-1.032977
H	-1.288753	0.707330	1.462582
H	-3.243743	0.280707	-0.392339

Frequencies:

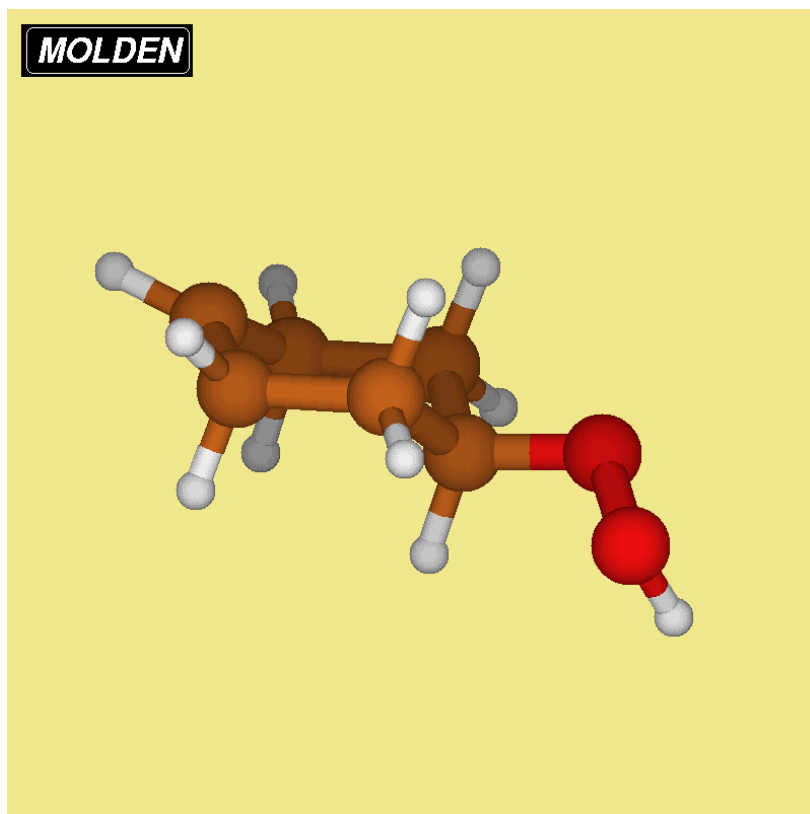
89.2396	135.6677	156.6029
202.1137	260.2735	296.5470

333.9506	371.0678	421.7342
517.4436	566.2373	688.3942
804.2898	821.3907	858.6234
875.4886	885.9932	941.8228
967.9399	1012.2724	1042.5753
1067.3094	1108.5034	1124.1968
1146.9328	1196.6274	1255.8220
1281.7878	1334.0749	1346.6796
1358.5240	1363.9345	1373.4888
1389.4420	1407.0884	1414.7051
1466.8675	1480.1096	1496.3765
1508.8624	2912.0402	2930.1312
3012.7461	3032.0690	3050.8914
3068.0205	3076.6539	3097.7914
3105.7114	3191.2423	3754.1489

Rotational constants (GHZ):      3.34233    1.62251    1.34121

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cyC6OOH-3\_eq



C	0.05044	0.07747	0.04034
C	-0.05841	1.60317	0.05277
C	0.07585	2.15179	1.4889

C	-0.81388	1.4313	2.4524
C	-0.92244	-0.05904	2.37176
C	-1.02921	-0.5638	0.91642
H	-1.0364	1.8761	-0.36165
H	-1.77783	-0.42141	2.95344
H	-0.94042	-1.65464	0.87877
H	0.70726	2.03243	-0.59921
H	-2.00977	-0.29988	0.50319
H	-0.03138	-0.52674	2.83386
H	-1.1576	1.94101	3.34838
H	-0.12622	3.22892	1.50088
O	-0.15683	-0.47273	-1.26517
O	0.93454	-0.01715	-2.11822
H	1.04786	-0.22814	0.39727
H	1.1326	2.04733	1.80381
H	1.41152	-0.85505	-2.23477

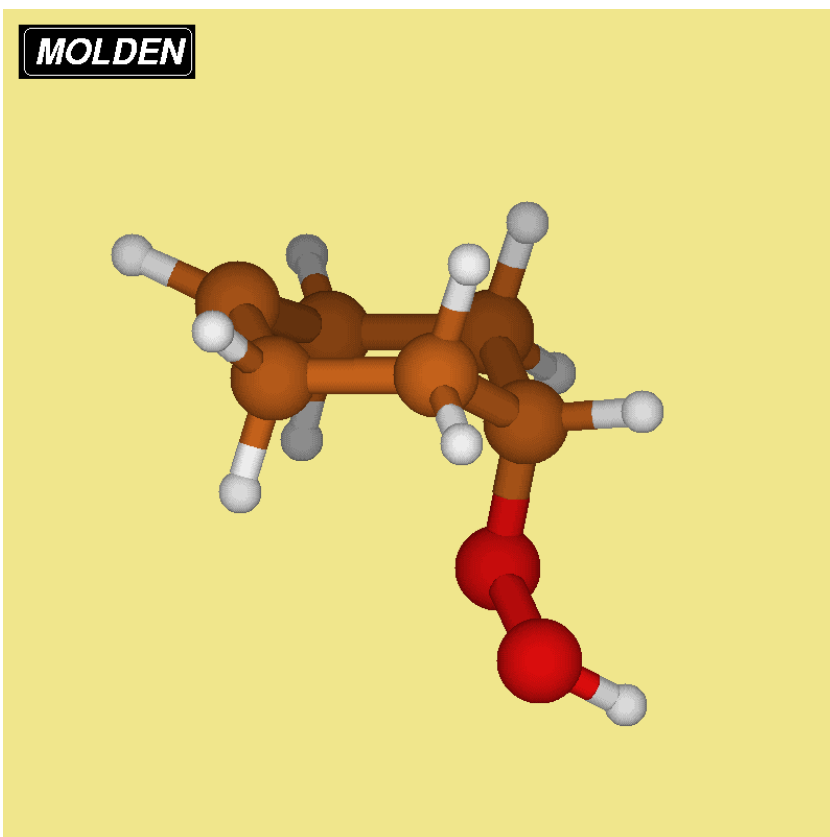
Frequencies:

104.3744	137.6049	202.9796
207.5152	212.8176	274.2279
367.6500	395.4559	443.8512
477.8667	516.0581	648.2319
782.9425	819.4199	874.8810
906.3512	929.3165	951.3241
965.2785	1023.6386	1064.3918
1084.5887	1104.7870	1116.6588
1143.3261	1219.3166	1251.4883
1285.3965	1315.3822	1330.8690
1345.7908	1360.2364	1372.4159
1393.9688	1398.1784	1414.3665
1478.9519	1485.2531	1501.4633
1519.1515	2919.3069	2924.1528
2984.4903	3049.4968	3053.9121
3068.6851	3070.0281	3099.0079
3114.8280	3183.3589	3753.7323

ROTATIONAL CONSTANTS (GHZ)      3.96037    1.39011    1.09843

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cyC6OOH-3\_ax



C	1.398072	-0.205930	-0.765909
C	0.046428	0.148975	-0.133170
C	-0.018861	-0.259379	1.342015
C	1.146518	0.335274	2.158483
C	2.469328	0.111950	1.495820
C	2.593178	0.366947	0.026481
O	-0.074197	1.570930	-0.307893
O	-1.389656	1.971582	0.171432
H	0.017474	-1.355542	1.385570
H	3.529495	-0.046844	-0.366133
H	1.420691	0.144658	-1.803457
H	-0.980535	0.051598	1.759777
H	1.463858	-1.300260	-0.790659
H	2.639598	1.454276	-0.162755
H	3.369185	0.051254	2.102214
H	1.141167	-0.077462	3.173825
H	-0.766210	-0.337996	-0.692718
H	-1.818304	2.176934	-0.675594
H	0.961115	1.418588	2.268990

Frequencies:

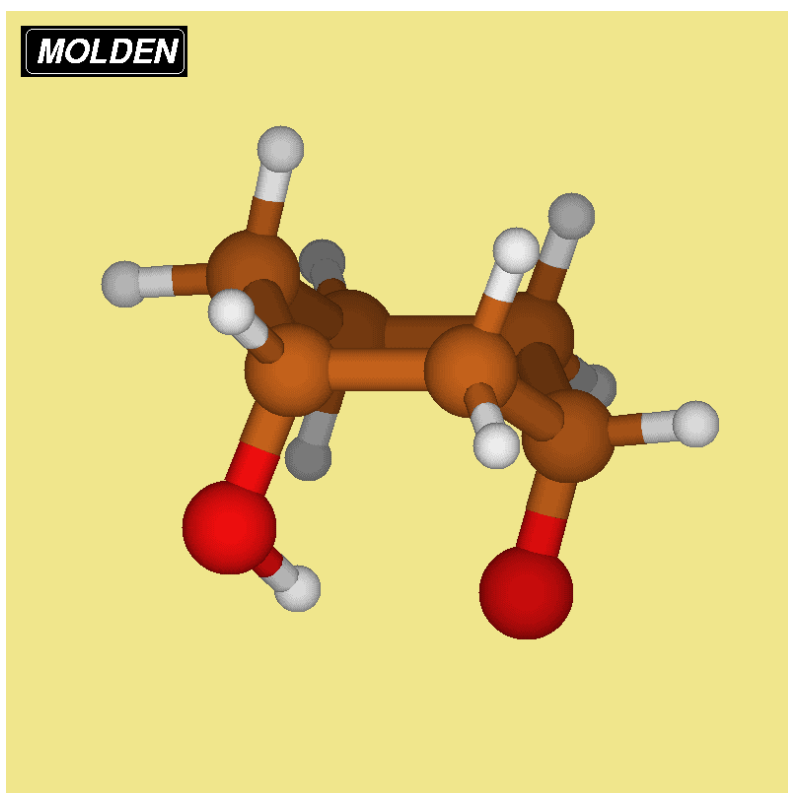
88.3245	144.3389	169.4909
208.6876	237.9706	297.8311

363.2858	388.9173	416.1052
535.2021	573.9932	684.5233
768.8164	812.4448	862.4283
880.6214	915.1802	953.5929
959.0247	1015.0098	1034.4207
1070.5799	1102.9224	1127.9629
1161.7358	1193.2994	1235.8631
1303.3207	1333.6762	1344.4589
1355.5927	1357.7229	1375.2654
1395.3040	1402.8441	1411.4721
1476.7342	1485.7459	1488.2925
1501.7061	2954.2705	2958.8036
3005.3765	3042.5954	3049.9698
3064.7012	3068.7143	3093.3424
3108.7294	3179.4172	3751.4622

Rotational constants (GHZ):      3.21070    1.67096    1.38122

\*\*\*\*\*

cyC6O\_OH-2\_ax



C 0.3309850294 -0.637615141 -1.5681843931  
C -1.015581517 -0.1304877199 -1.0054763332  
C -1.1847648047 -0.6133614501 0.4924289986



C 0.0066619117 -0.1756834079 1.3551208525  
C 1.3418056745 -0.6543985392 0.7577500496  
C 1.5183964493 -0.2051800372 -0.7001505752  
O -1.0900883699 1.2339500243 -0.948226886  
O -0.0118868864 1.2268030149 1.5793113417  
H -1.2732704079 -1.705663532 0.4537975322  
H 1.3806224659 -1.7515643017 0.812808821  
H 2.4488387035 -0.6119513652 -1.1108143069  
H 0.4420631428 -0.2694495036 -2.5940230841  
H -2.1132493068 -0.2028491207 0.8966619985  
H 0.2776565165 -1.7334170769 -1.6266516483  
H 1.6129738388 0.8859731186 -0.7381739761  
H 2.1565640704 -0.2708954724 1.380379827  
H -0.1161252709 -0.627279382 2.3485228173  
H -1.8659757869 -0.5515246184 -1.5714719243  
H -0.1193123749 1.6529547129 0.7113567035

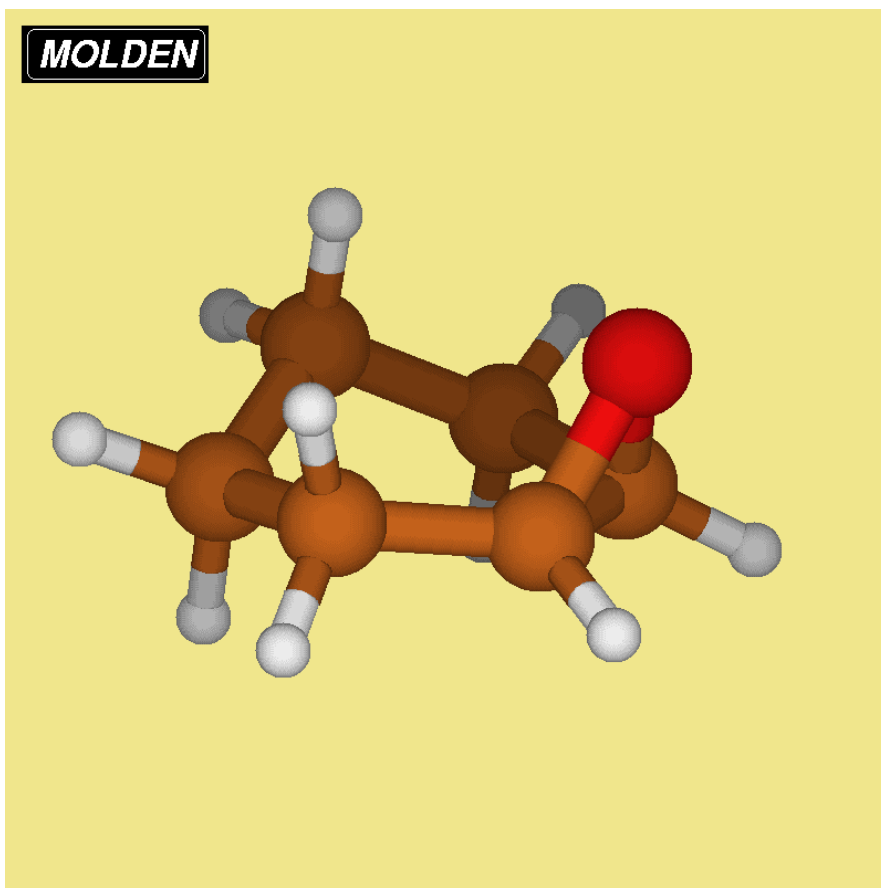
Frequencies:

139.3782	182.7068	270.4634
324.5616	358.3231	390.0230
422.1200	481.4062	516.1276
592.2770	699.5093	745.0548
814.0849	840.4079	857.2853
888.2360	934.9684	982.7706
1002.2902	1018.0052	1066.7266
1073.2590	1098.5739	1139.5994
1177.1680	1233.0502	1262.7283
1275.2497	1289.4418	1322.5510
1346.4667	1357.7140	1378.6541
1396.5629	1415.8851	1440.9119
1474.3993	1488.1827	1500.9989
1511.5371	2950.8108	3023.1380
3032.0024	3038.6171	3055.6242
3059.4536	3085.8499	3092.1970
3098.7361	3127.1436	3688.3861

Rotational constants (GHZ): 2.57542 2.27348 1.69121

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epoxyxyC6-1



C	0.80975	0.99417	1.90079
C	1.07209	0.80327	3.34135
O	0.45169	2.00593	2.86388
C	1.92137	1.36226	0.93072
C	2.47027	0.95022	3.90247
C	3.3289	1.2483	1.54436
C	3.37901	1.77998	2.98291
H	-0.05637	0.49051	1.46717
H	0.40134	0.15196	3.90688
H	1.84862	0.72374	0.04241
H	1.73708	2.38956	0.59188
H	2.41385	1.39995	4.90178
H	2.89057	-0.05685	4.03472
H	3.6373	0.19361	1.54889
H	4.0499	1.77862	0.91214
H	3.05453	2.82664	3.00278
H	4.4064	1.75414	3.36267

Frequencies:

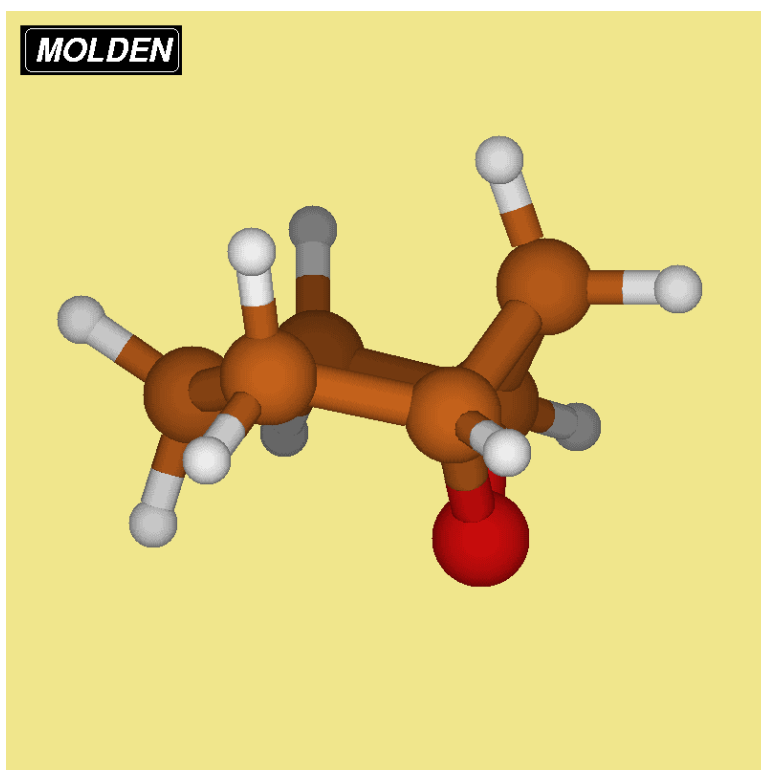
145.3403	271.4111	356.5468
373.9955	441.7841	543.9893
648.4661	775.8320	787.8321

830.3086	851.7892	897.7471
906.7088	990.2551	1008.3653
1044.5515	1057.1959	1081.5638
1102.0913	1167.6417	1198.7304
1218.7313	1279.8129	1293.5352
1308.6521	1359.2881	1381.0137
1387.6181	1396.8055	1407.2095
1476.2569	1492.7049	1496.2942
1502.1422	1514.0707	3023.8173
3025.6937	3039.6952	3049.6628
3066.8727	3074.4884	3084.0230
3096.1548	3097.3743	3112.6995

ROTATIONAL CONSTANTS (GHZ)      3.84853    3.14532    2.09697

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epoxyxyC6-2



C	0.16331	0.02246	-0.12621
C	-0.1068	-0.54918	1.27782
C	0.83084	0.59851	1.69558
C	2.30304	0.17262	1.60489
C	2.66201	-0.09197	0.119
C	1.44929	-0.56506	-0.72495

H	0.20083	-1.5776	1.49032
H	2.45763	-0.717	2.22865
H	3.49471	-0.79752	0.03721
H	1.57722	-0.23776	-1.76256
H	-1.13637	-0.38377	1.60293
H	1.36684	-1.65929	-0.74598
H	3.00857	0.85268	-0.30695
H	2.95666	0.956	2.004
H	0.59432	1.17212	2.59711
H	-0.66459	0.0855	-0.83917
O	0.46879	1.3241	0.47454

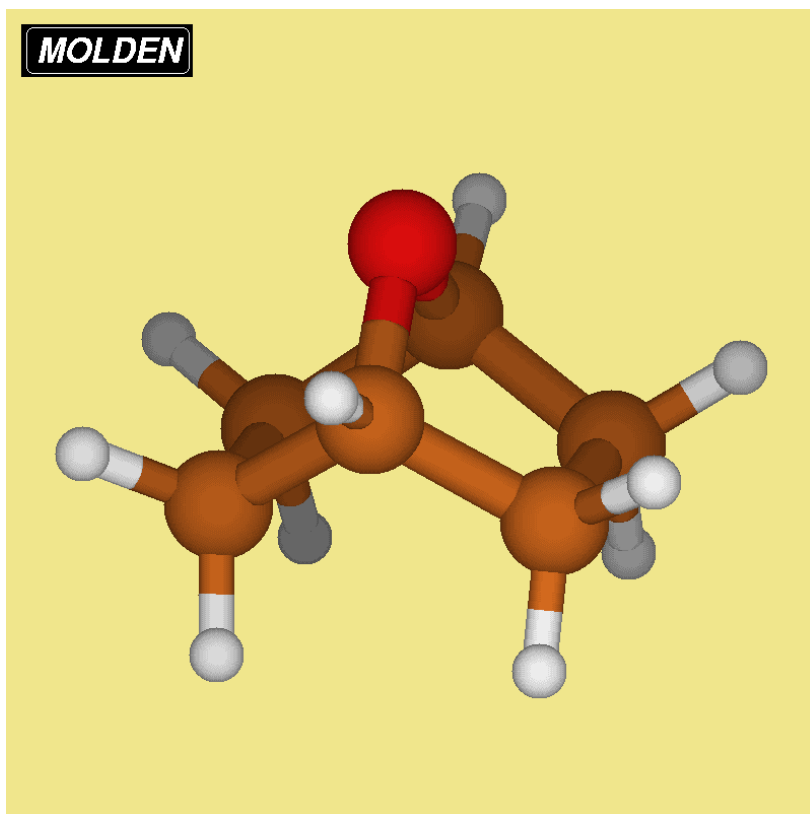
Frequencies:

146.4297	296.4960	395.4158
427.4851	543.7642	620.9653
760.3827	813.2850	827.6413
857.5641	875.4448	922.3557
937.7176	957.6162	987.2909
1028.4379	1037.8977	1092.9090
1121.3859	1125.4911	1158.9554
1232.9274	1242.5893	1266.1967
1273.7762	1336.9437	1339.0366
1353.4684	1359.4092	1386.4271
1388.2319	1492.5631	1503.6831
1505.1876	1521.7001	3038.9777
3039.7766	3067.7290	3070.5322
3078.3984	3080.1039	3087.2257
3089.3695	3117.5325	3135.6242

ROTATIONAL CONSTANTS (GHZ)      3.93460    3.30710    2.56156

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epoxyxyC6-3



C	0.52848	0.2762	0.00807
C	1.34795	1.32707	0.79139
C	0.20884	2.14029	1.4797
C	-1.04226	1.39821	0.95579
C	-1.18525	0.03257	1.66625
C	-0.04466	-0.7806	0.97998
H	1.92397	1.95394	0.10565
H	-2.16502	-0.40636	1.46042
H	0.70455	-1.15378	1.68433
H	2.04579	0.87312	1.50122
H	-0.44373	-1.63518	0.42733
H	-1.0698	0.10854	2.75145
H	-1.95337	1.99662	0.90614
H	0.20601	3.1809	1.14479
O	-0.6451	1.01767	-0.37565
H	1.01409	-0.1244	-0.88331
H	0.27403	2.1371	2.57177

Frequencies:

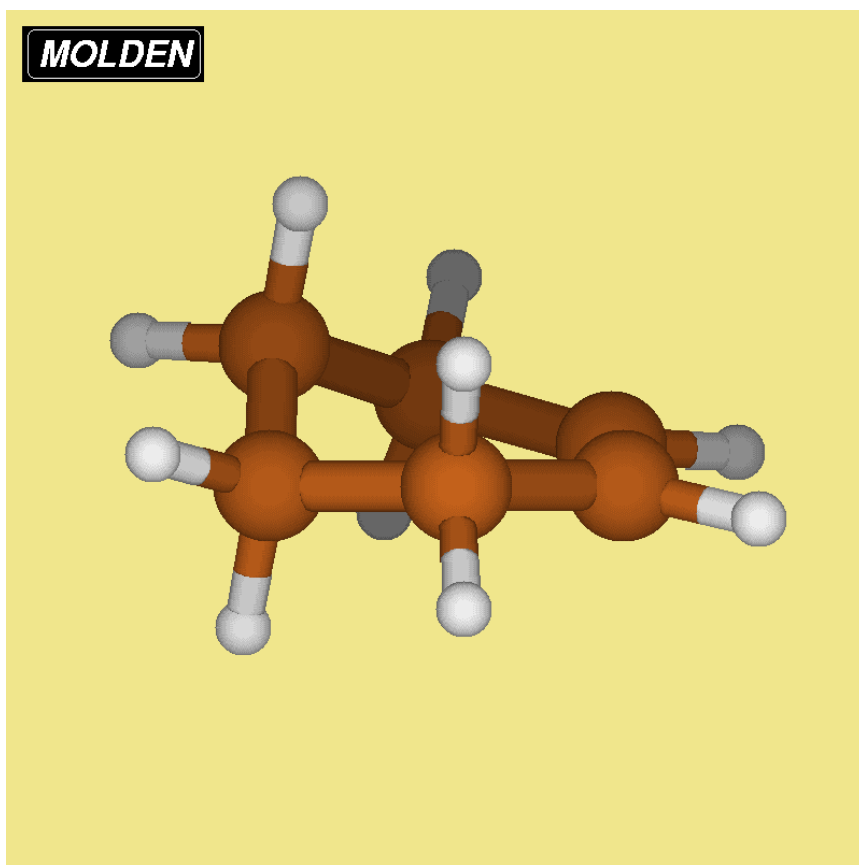
140.6553	318.3479	394.7762
550.9903	583.9450	764.3822
801.4982	813.0192	832.6873
836.7062	891.7509	917.6284
935.5187	959.9029	983.4981

1014.1186	1026.1552	1029.1997
1100.6638	1128.4932	1182.2585
1229.5816	1235.8892	1236.8373
1281.8252	1301.7880	1305.7017
1316.2345	1339.9109	1355.5935
1367.5734	1489.7115	1502.0622
1511.2373	1526.8134	3065.8556
3069.1513	3075.0029	3078.7540
3107.4439	3110.5072	3124.2842
3128.3103	3129.0551	3135.4836

ROTATIONAL CONSTANTS (GHZ)      3.92197    3.28492    2.83085

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cyC6H10



C	0.58502	1.19876	-0.69304
C	0.89814	0.79486	0.75642
H	1.50518	1.50724	-1.20674
H	-0.06681	2.08616	-0.70513
C	-0.28681	0.05094	1.38773
H	1.77842	0.13832	0.76505

H	1.15962	1.67965	1.34806
H	-0.07999	-0.18624	2.4376
H	-1.16708	0.7075	1.38032
C	-0.60929	-1.2329	0.60681
C	-0.59353	-1.00753	-0.88546
H	-1.58919	-1.62418	0.91105
H	0.11256	-2.02339	0.86482
C	-0.07631	0.08148	-1.46267
H	-1.03488	-1.78435	-1.50807
H	-0.12115	0.18565	-2.54573

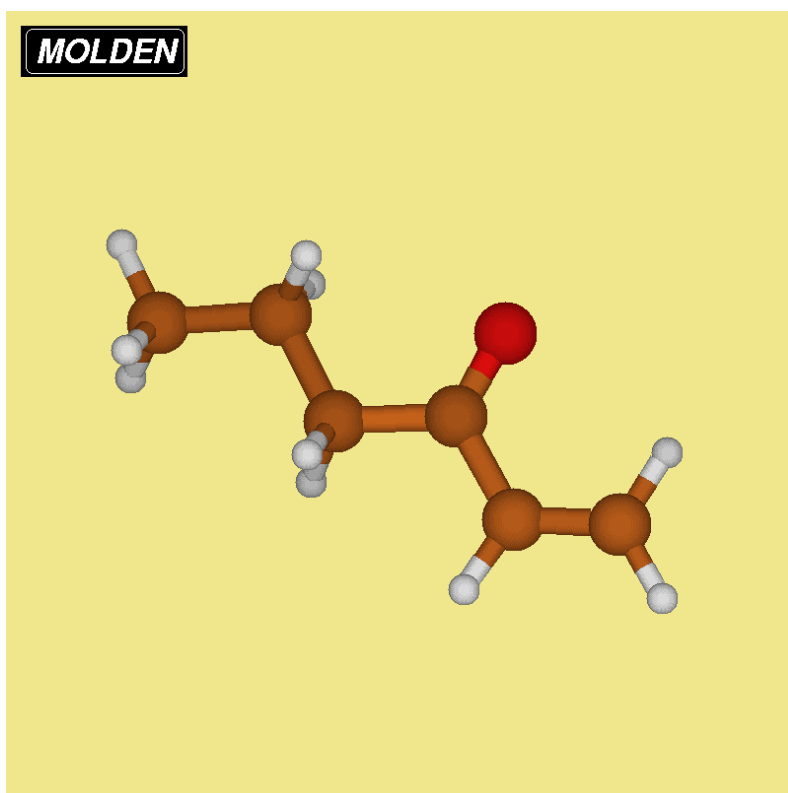
Frequencies:

165.8955	279.5317	397.5154
457.2065	501.7144	655.4996
732.8075	826.0442	831.4504
885.8279	913.7535	939.1310
1002.1684	1020.0256	1051.1760
1075.8183	1100.1677	1165.4276
1165.4519	1253.7169	1274.5453
1297.8746	1357.1976	1380.7301
1383.2987	1393.2327	1429.1919
1486.8259	1493.0084	1505.4502
1515.7206	1734.4194	3002.6933
3002.9181	3028.4729	3031.5171
3048.2491	3048.7440	3076.6678
3081.9539	3144.6328	3168.1389

ROTATIONAL CONSTANTS (GHZ)      4.71660    4.52862    2.54250

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1-Hexen-3one C6H10O



C	-1.36901	0.35864	-2.88178
C	-1.30804	0.14984	-1.36651
H	-2.40441	0.37625	-3.23615
H	-0.90271	1.30637	-3.17503
H	-0.84921	-0.44359	-3.41832
C	0.12213	0.1182	-0.83004
H	-1.86227	0.94297	-0.85263
H	-1.8105	-0.78445	-1.09277
H	0.70814	-0.67759	-1.31563
H	0.6567	1.04873	-1.07674
C	0.21929	-0.08709	0.67442
C	1.60138	-0.12493	1.24673
C	1.80732	-0.29913	2.55477
O	-0.77151	-0.21395	1.37718
H	2.43482	-0.00501	0.55743
H	2.80383	-0.32849	2.9837
H	0.95928	-0.41682	3.22322

Frequencies:

62.0545	72.0906	131.8819
145.2958	247.1148	297.7143
334.3043	422.5034	463.0646
652.9325	660.2671	759.7966
841.4715	893.8908	912.4248

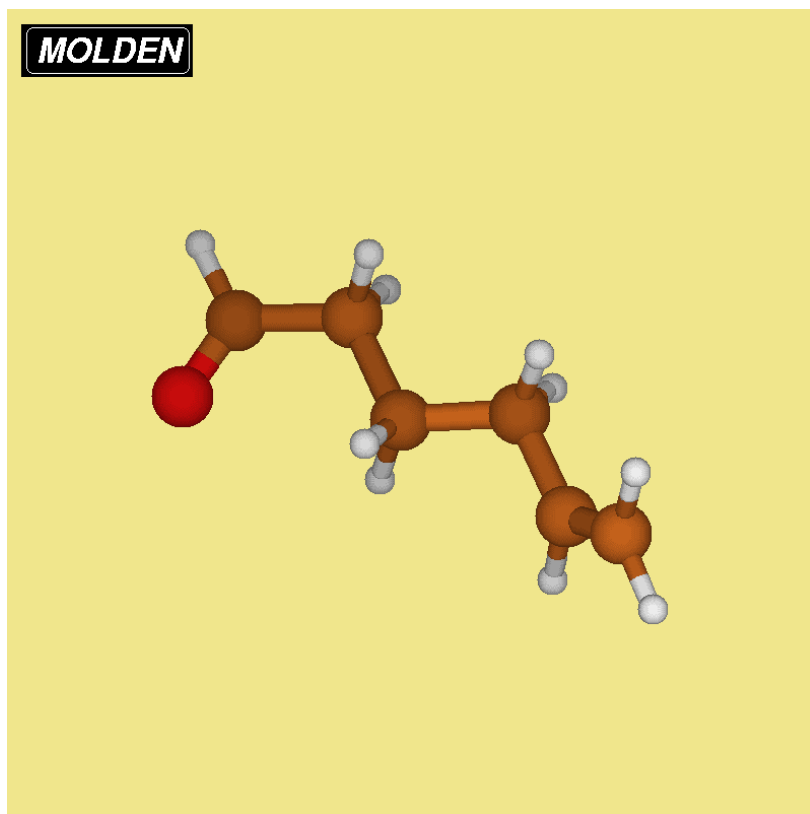


999.9260	1032.3530	1050.4013
1066.0734	1089.5147	1108.1905
1150.6684	1252.4958	1316.5821
1326.7888	1336.8922	1406.8808
1429.2993	1443.0492	1465.7528
1501.5623	1514.7131	1521.5329
1688.2818	1789.8380	3006.9589
3033.8785	3036.2823	3059.4529
3086.0023	3109.9212	3113.7750
3160.3769	3174.4882	3257.9171

ROTATIONAL CONSTANTS (GHZ)      8.28362   1.18642   1.05794

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5-hexenal



C	-1.35724	0.09065	-2.31543
C	-1.35051	0.18386	-0.80731
H	-2.36897	0.14264	-2.77985
C	0.03889	0.09554	-0.17697
H	-1.85625	1.12492	-0.53883
H	-2.01757	-0.60667	-0.42926
H	0.5067	-0.85345	-0.46009

H	0.67503	0.88006	-0.60316
C	0.00728	0.22131	1.35674
C	1.37919	0.17593	1.97228
C	1.79606	-0.72857	2.85782
H	2.07206	0.95142	1.64196
H	2.80347	-0.7105	3.26268
H	1.14233	-1.52148	3.21417
H	-0.61473	-0.57497	1.78533
H	-0.47806	1.17293	1.62247
O	-0.36826	-0.02966	-3.00478

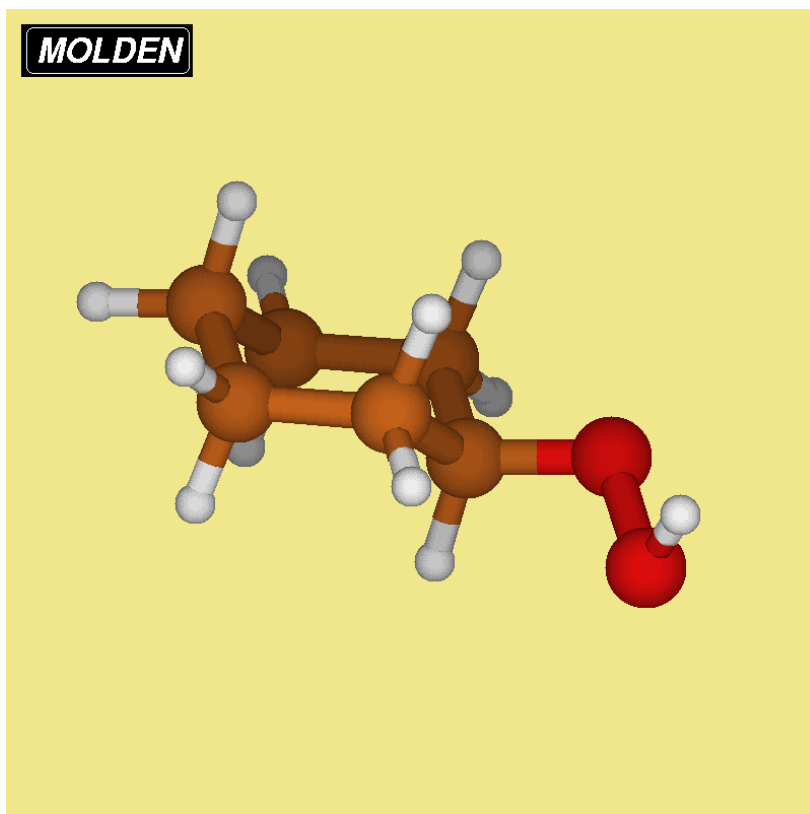
Frequencies:

55.6834	87.2113	102.4442
149.1188	179.1971	268.1856
355.6361	436.8084	632.5266
673.6778	715.8395	778.1630
892.4272	921.4460	943.1882
952.5705	1030.4703	1044.3744
1048.1223	1086.5010	1162.7724
1217.6085	1266.3857	1297.8565
1323.2582	1333.6791	1361.2783
1405.9152	1428.5341	1461.8977
1466.2956	1494.4691	1512.5232
1730.8776	1831.0223	2882.9617
3004.7086	3008.7359	3033.3095
3054.4687	3060.0944	3101.5166
3135.5337	3150.2853	3234.0803

ROTATIONAL CONSTANTS (GHZ)      8.49883    0.95712    0.90071

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cyC6H11O2H - cyclohexyl-hydroperoxide



c	0.0136	-0.01905	-0.06737
c	-0.04344	-0.05816	1.46275
c	1.36057	0.09052	2.07068
c	2.32381	-0.97148	1.5192
c	2.36203	-0.94813	-0.0167
c	0.95617	-1.08974	-0.62432
h	-0.48015	-1.02029	1.76532
h	1.99733	-1.96495	1.85732
h	3.00892	-1.74753	-0.39558
h	0.99057	-1.0145	-1.71608
h	-0.709	0.73248	1.8237
h	0.54412	-2.07828	-0.38218
h	2.80785	-0.00197	-0.35346
h	3.33095	-0.81898	1.92457
h	1.30421	0.02681	3.16339
o	-1.25547	-0.28737	-0.6737
o	-2.12574	0.84872	-0.38937
h	0.35058	0.97437	-0.39851
h	1.75232	1.09088	1.83882
h	-2.7842	0.4182	0.1792

Frequencies:

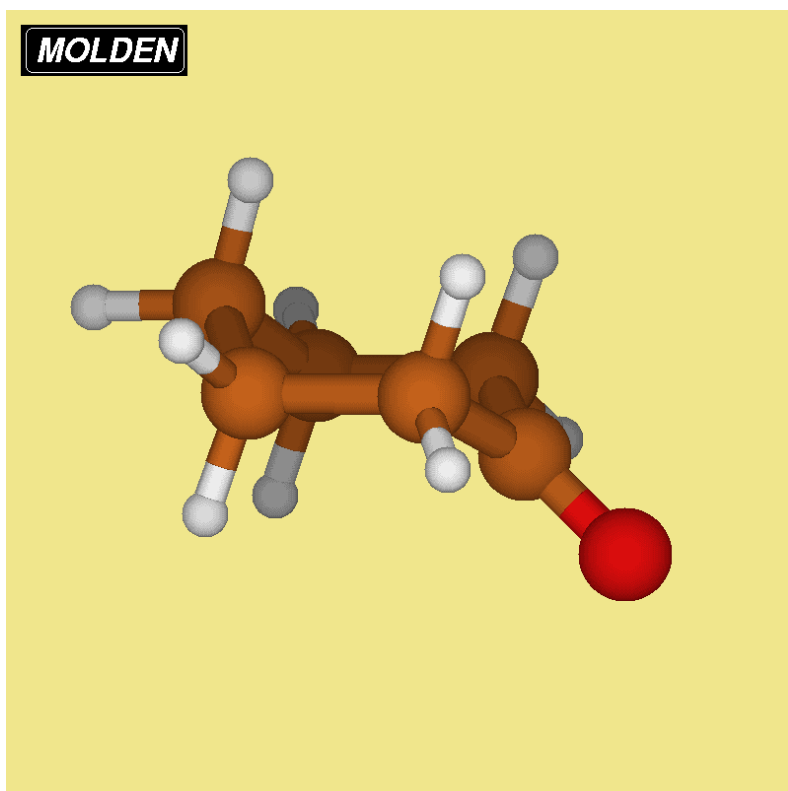
103.2822	148.3736	223.0139
232.7253	244.7188	330.6099
368.6200	439.4947	467.9445

490.4781	559.9673	799.1703
806.6048	849.6602	897.4066
899.8201	929.1092	944.2932
976.1837	1031.4448	1065.0490
1080.5066	1093.0271	1108.5034
1179.0589	1210.8652	1275.6784
1284.7211	1290.5721	1331.0174
1341.9045	1362.0335	1372.9134
1387.3524	1388.7305	1398.1679
1408.4227	1497.6972	1499.1025
1504.2399	1509.2065	1523.8777
3013.6058	3022.9944	3024.5277
3028.8688	3031.2127	3040.9370
3074.4493	3076.5584	3081.7589
3094.3851	3097.3004	3764.6036

ROTATIONAL CONSTANTS (GHZ)      3.94115    1.35062    1.08239

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cyclo-Hexanone



C	0.07942	1.9569	0.0853
C	-0.00815	0.45946	-0.17276

C	0.05171	-0.35775	1.13659
C	1.25302	0.04609	2.00335
C	1.23579	1.55054	2.31149
C	1.1961	2.39736	1.02099
O	-0.69123	2.75174	-0.42743
H	0.8516	0.18647	-0.80351
H	2.18572	-0.21048	1.47999
H	2.11103	1.83284	2.90793
H	1.07576	3.46369	1.23067
H	-0.91757	0.25658	-0.74484
H	2.14565	2.26814	0.47954
H	0.35312	1.78594	2.92161
H	1.25123	-0.52799	2.93759
H	-0.87548	-0.19514	1.70283
H	0.08818	-1.42699	0.89841

Frequencies:

92.8503	187.3565	306.5933
404.4207	417.2061	480.6587
490.8017	653.6997	751.7039
763.9325	841.0489	875.7540
896.8463	918.6457	999.7126
1025.5515	1063.1227	1079.6713
1136.8005	1137.3387	1241.6333
1248.3193	1273.6910	1288.8067
1339.4999	1348.0868	1367.1397
1381.3127	1382.0864	1468.5169
1474.8342	1496.6646	1497.6887
1512.3895	1786.2532	3013.0288
3016.4554	3019.5322	3029.9799
3031.7511	3071.5611	3075.3584
3079.6011	3112.2769	3113.6166

Rotational constants (GHZ): 4.19077 2.46854 1.72669

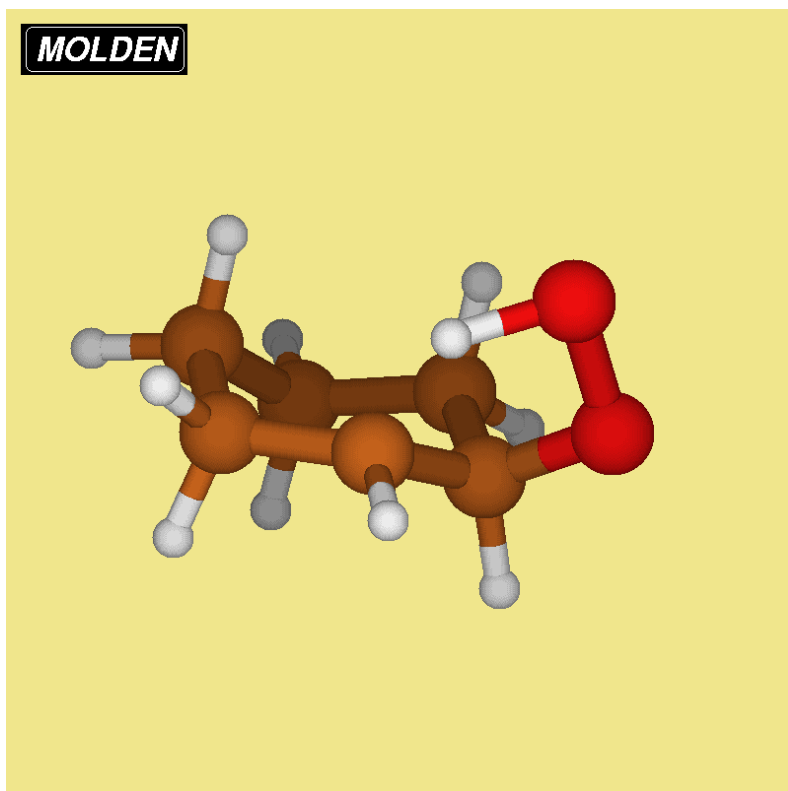
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Transition state structures

all structures optimized at the b3lyp/6-31g(d,p) level  
and used as input for g2mp2 calculation

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cyC6OO\_eq->cyC6OOH-1\_eq



c	0.71731	0.3279	-0.70189
c	0.23983	-1.10795	-0.42228
c	-1.23054	-1.37517	-0.23457
c	-1.96046	-0.2592	0.52836
c	-1.61745	1.11959	-0.05196
c	-0.10751	1.38776	0.03857
h	1.0571	-1.0552	0.67837
h	-1.66926	-0.28677	1.58663
h	-2.16383	1.90473	0.48224
h	0.14269	2.37859	-0.35495
h	0.77046	-1.85547	-1.01934
h	0.20215	1.36648	1.08868
h	-1.94964	1.16931	-1.0993
h	-3.04116	-0.43626	0.4937
h	-1.37702	-2.35002	0.24798
o	2.08917	0.29002	-0.26397
o	1.99845	-0.34753	1.01052
h	0.76654	0.54444	-1.77824
h	-1.68604	-1.4772	-1.2356

Frequencies:

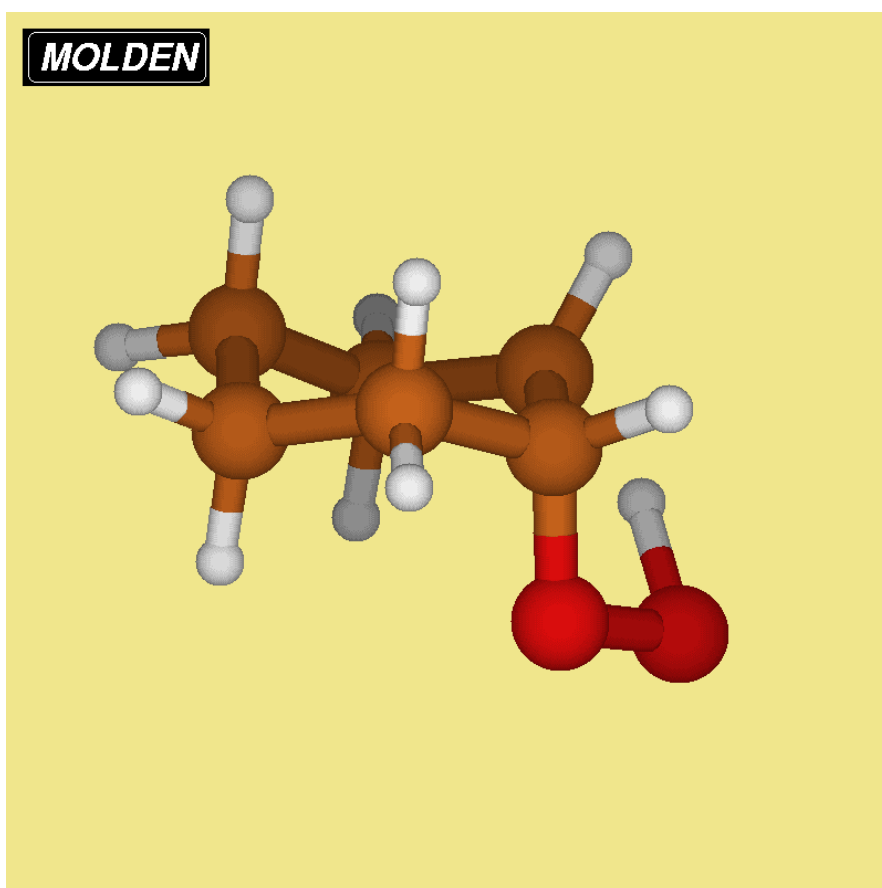
-2135.7736	123.4553	179.7917
273.7111	322.1500	378.6838
415.7029	476.7498	527.4923

573.1052	703.7465	780.9554
794.7941	855.1394	885.5154
898.1869	919.2771	936.4052
947.2468	1013.2923	1047.5781
1064.8364	1107.7329	1130.4566
1148.6213	1173.1460	1206.0916
1265.2582	1277.2636	1307.0219
1341.5170	1350.8380	1375.0968
1387.3633	1390.3411	1404.7272
1470.4773	1498.9920	1504.8345
1514.5574	1724.7167	2966.5452
3018.9542	3034.4105	3035.6681
3055.0740	3058.9424	3080.5973
3084.7321	3105.1260	3108.9525

ROTATIONAL CONSTANTS (GHZ)      3.42018    1.65734    1.36523

\*\*\*\*\*

cyC6OO\_ax->cyC6OOH-1\_ax



C 0.6908757018 -0.5546155372 0.612880895  
C -0.5229474534 -1.4707826797 0.4491227401

C -1.5707451961 -0.9011372298 -0.518718838  
C -1.9671833703 0.5314628028 -0.1366324329  
C -0.7300693211 1.4624884691 -0.1436398058  
C 0.3463352769 0.9359287903 0.7798025907  
H -0.9691563325 -1.603985587 1.4433514587  
H -2.4284374338 0.5368384325 0.8605180426  
H -1.0102954717 2.4833760613 0.1343749234  
H 1.5662530706 1.176525437 0.2182996355  
H -0.1788237187 -2.4596330127 0.1243298777  
H 0.3137021771 1.3001038241 1.8087294796  
H -0.3435181446 1.496856401 -1.1700030926  
H -2.7170690776 0.9218178511 -0.8342611261  
H -2.4532972102 -1.5509498924 -0.526491088  
H -1.1637822388 -0.9048588199 -1.5367430948  
H 1.3285142789 -0.8801881817 1.4458518714  
O 1.4590193793 -0.5768631264 -0.6049033766  
O 2.3632701551 0.5098668507 -0.4232025962

Frequencies:

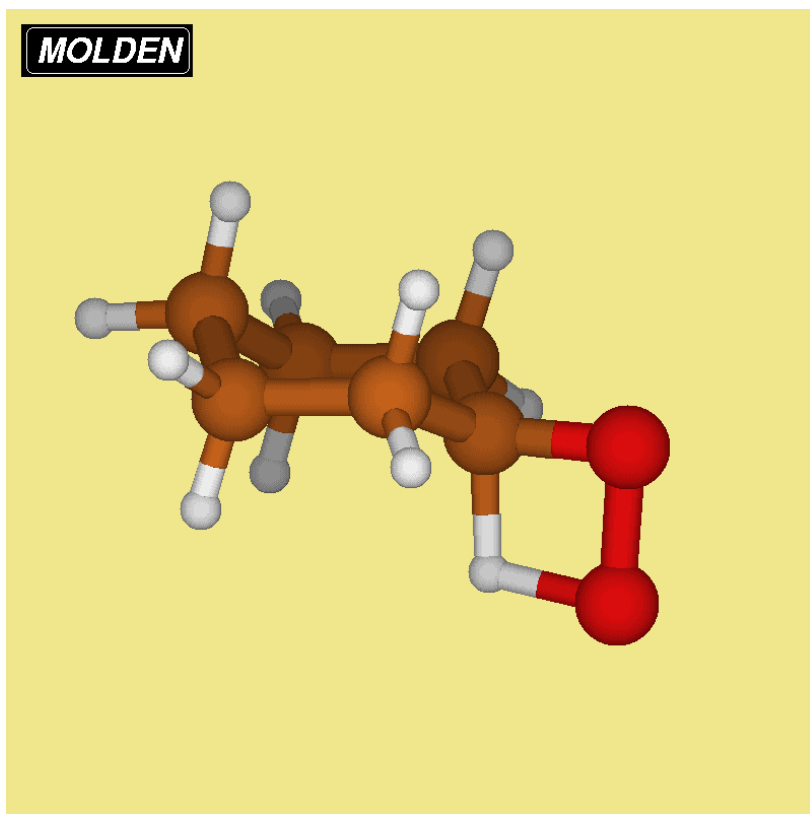
-2121.1456	140.5665	167.7182
250.6398	297.3353	352.8005
431.4250	459.6612	580.2063
622.0319	691.6956	781.1056
820.5489	839.2504	867.0788
894.2013	919.5131	943.5970
965.9532	1007.0835	1039.9456
1052.7532	1091.1328	1139.3875
1143.0572	1171.0453	1198.1713
1276.2923	1292.5145	1336.4283
1341.3066	1355.7396	1364.7531
1386.1034	1396.5918	1399.9821
1485.0607	1495.6195	1502.1772
1512.3014	1720.8788	3027.7619
3028.4880	3042.1056	3043.1424
3047.5828	3078.7866	3082.3983
3093.4421	3096.6827	3130.1498

Rotational constants (GHZ): 3.30231 1.78531 1.41552

\*\*\*\*\*

cyC6OO\_eq --> cyC6H10O + OH





```
C -0.7140144279 0.0001913901 0.1483806436
C 0.0418650523 1.2934288191 0.3684530253
C 1.4163598547 1.2696991195 -0.3213619015
C 2.2056790789 -0.0001071564 0.0326923415
C 1.416338654 -1.2697603086 -0.3219693236
C 0.0412745204 -1.2936726305 0.3668347709
H 0.1721336566 1.4134256845 1.4560377035
H 2.4317529593 -0.0003661623 1.1084348652
H 1.9833473276 -2.1651453416 -0.0447264815
H -0.5717611267 -2.1350576711 0.0292739525
H -0.5710194224 2.1357111721 0.0328787068
H 0.1705545695 -1.4156830265 1.4542993637
H 1.2743775697 -1.3142799465 -1.410269618
H 3.1697910827 -0.000010945 -0.4882216012
H 1.9836308471 2.1650729437 -0.0446350382
O -2.0308080871 0.0001307707 0.6281808232
O -2.5297186687 0.0001885999 -0.7866522539
H -1.2771040014 0.0009673196 -1.0539220948
H 1.2734941893 1.3141356101 -1.4095556506
```

Frequencies:

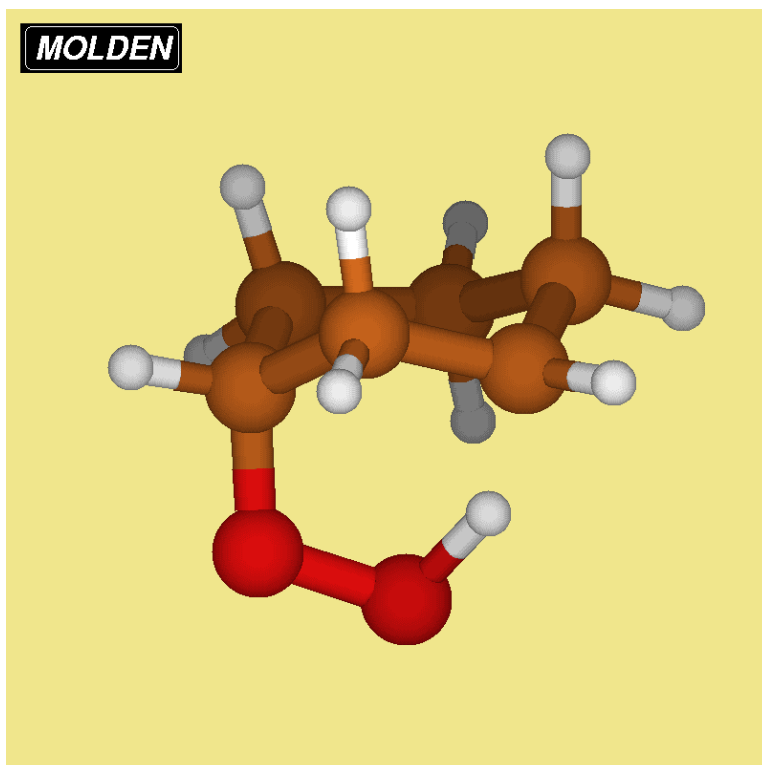
-1770.9788	104.4900	113.3250
226.2836	282.9000	354.6761

360.5129	436.5522	449.2529
552.9884	649.0568	784.8491
815.7742	835.0211	850.2993
900.6466	904.5669	919.2699
984.0582	996.9838	1031.4493
1081.6245	1102.6664	1125.8792
1157.6655	1167.8915	1246.2931
1272.0148	1288.8900	1303.9454
1349.6391	1375.2428	1377.6436
1389.0147	1394.8099	1476.5559
1485.8428	1499.9113	1502.8960
1516.9764	1953.4286	2997.5365
3002.7349	3023.9352	3032.7480
3035.8840	3080.9976	3083.6089
3087.3086	3097.0350	3098.0987

Rotational constants (GHZ):      3.65959    1.47388    1.21835

\*\*\*\*\*

cyC6OO\_ax->cyC6OOH-2



c	-0.88769	0.39743	0.7908
c	0.20341	1.44888	0.52835
c	1.31496	1.0135	-0.45116
c	1.7831	-0.44504	-0.23452

c	0.61021	-1.37936	-0.00892
c	-0.26583	-0.9714	1.14811
h	0.64632	1.67844	1.50752
h	2.43888	-0.49442	0.65139
h	0.79246	-2.44718	-0.14056
h	-1.06117	-1.69693	1.34135
h	-0.2694	2.37075	0.17363
h	0.3253	-0.86206	2.07135
h	-0.29794	-1.01609	-0.99091
h	2.39179	-0.77162	-1.08464
h	2.17039	1.69187	-0.35432
h	0.93889	1.11016	-1.47131
h	-1.55663	0.74496	1.58631
o	-1.80038	0.16877	-0.29277
o	-1.0831	-0.25526	-1.44794

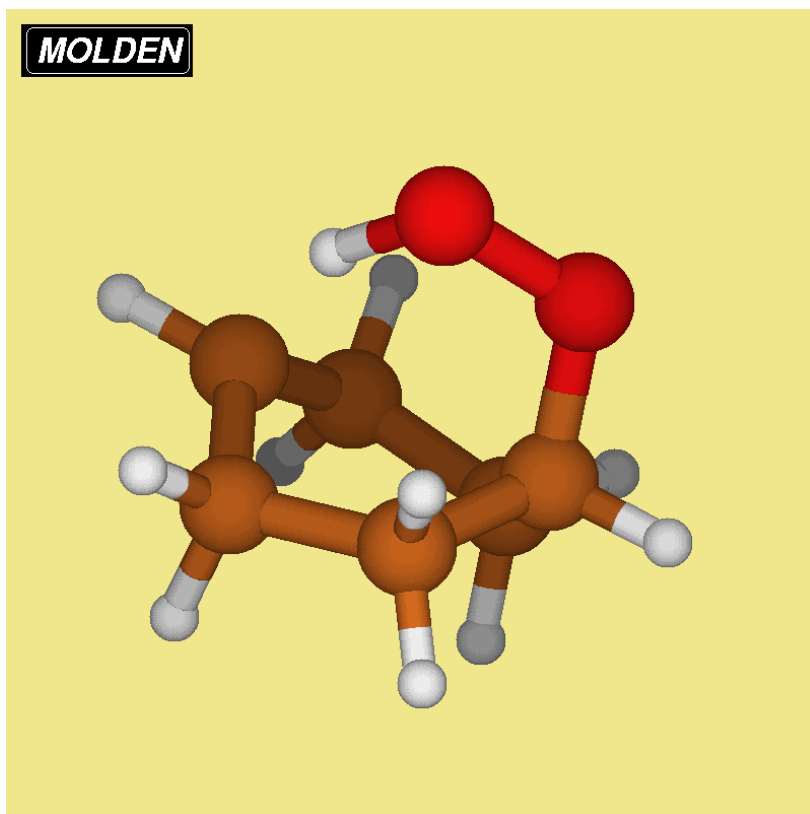
Frequencies:

-1714.0750	186.2936	223.9261
261.5214	370.8167	391.6449
423.1505	515.7168	536.1240
610.1608	731.9644	772.9504
791.7527	840.5917	880.9379
885.0884	909.0435	930.0348
988.2989	1027.5170	1038.1203
1060.9697	1083.9043	1128.2602
1138.2124	1157.7020	1211.7434
1240.4194	1286.5349	1313.0460
1339.1488	1350.2550	1363.3515
1375.7919	1388.3104	1405.5148
1474.2253	1485.2840	1494.0320
1510.5805	1577.5882	2976.7536
2996.7667	3028.3178	3057.4810
3074.8902	3078.6128	3090.4046
3102.6099	3129.5359	3132.1229

ROTATIONAL CONSTANTS (GHZ)      2.77048    2.04413    1.87721

\*\*\*\*\*

cyC6OO\_eq->cyC6OOH-3



C	-0.73622	0.46134	0.86172
C	0.43333	1.42806	0.63414
C	1.24546	1.02149	-0.62212
C	1.12145	-0.46542	-0.89703
C	1.00747	-1.34591	0.33386
C	-0.22583	-0.94703	1.19722
H	1.06978	1.41083	1.52833
H	1.73644	-0.84811	-1.7143
H	1.93029	-1.24429	0.92678
H	-1.04169	-1.65859	1.05553
H	0.05903	2.45073	0.53119
H	0.03948	-0.9613	2.25974
H	0.94344	-2.39976	0.04677
H	-0.17408	-0.56239	-1.33883
H	2.304	1.2949	-0.49508
H	0.89439	1.58362	-1.49509
H	-1.38876	0.8275	1.66267
O	-1.59067	0.49983	-0.32078
O	-1.34012	-0.60088	-1.18102

Frequencies:

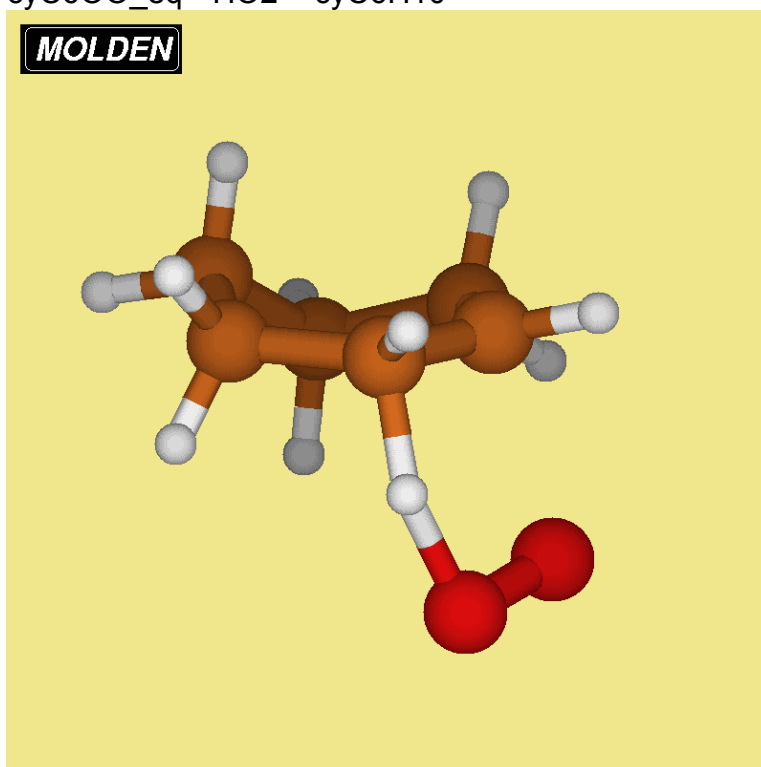
-1807.4082	132.3651	193.8167
266.6741	324.6550	340.6535
438.0120	491.0117	541.3257

634.4124	733.4202	773.5031
791.6140	824.9765	868.9568
890.8955	911.6409	927.6301
977.1278	1011.3986	1045.3366
1063.5992	1103.8534	1111.3396
1156.5601	1175.2173	1232.7129
1253.8515	1271.1689	1304.1598
1338.1835	1349.2392	1356.7132
1370.7392	1383.3794	1394.1111
1480.6390	1484.1931	1496.6379
1510.7010	1534.8805	2992.8965
3004.2834	3042.1187	3057.7875
3068.1417	3073.4362	3090.2076
3103.3642	3122.6301	3131.4337

ROTATIONAL CONSTANTS (GHZ):            2.53249    2.17529    2.00519

\*\*\*\*\*

cyC6OO\_eq->HO2 + cyC6H10



c	0.36521	0.37925	1.05621
c	0.16232	-0.97925	0.79544
c	-1.04152	-1.45068	-0.0402
c	-2.04204	-0.32208	-0.33767
c	-1.31937	0.97447	-0.72583

c	-0.46109	1.47189	0.44405
h	0.49873	-1.66693	1.5742
h	-2.6551	-0.13167	0.55402
h	-2.03815	1.74876	-1.01494
h	0.18252	2.30647	0.14471
h	1.21308	-1.07339	-0.01269
h	-1.11613	1.86711	1.23824
h	-0.67756	0.79427	-1.59767
h	-2.73049	-0.63461	-1.13065
h	-1.54722	-2.2654	0.49003
h	-0.6934	-1.88136	-0.98839
h	1.02224	0.66441	1.87312
o	2.11803	0.5989	-0.32561
o	2.20202	-0.62006	-0.70964

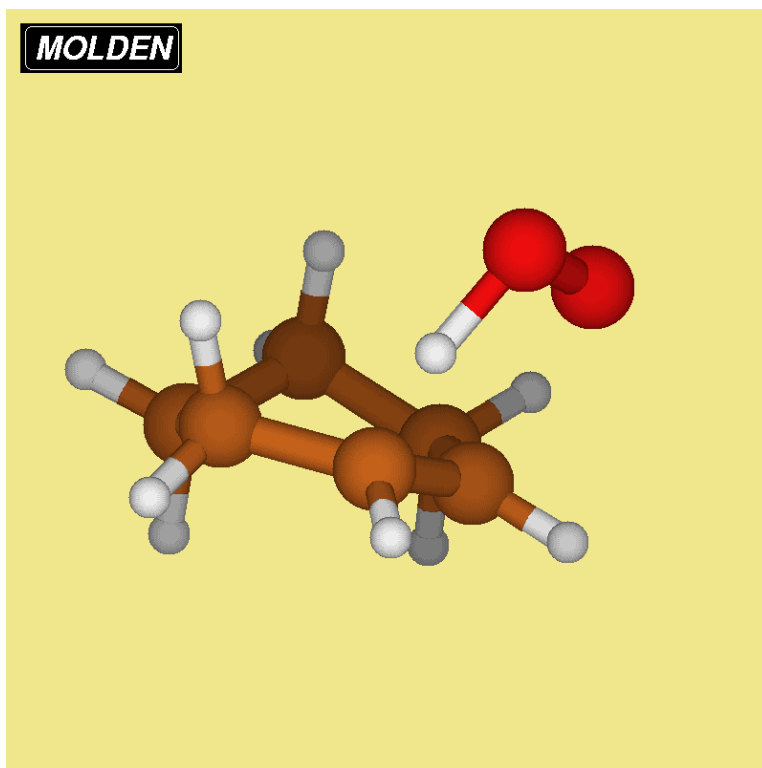
Frequencies:

-988.4217	83.2437	121.3588
195.7356	217.9193	312.0538
395.5025	443.2178	469.6227
542.7286	646.5240	712.0717
796.8275	819.6862	829.4360
888.0832	911.3666	946.3271
972.6830	1029.1322	1054.2250
1077.3803	1107.8751	1152.7932
1185.3275	1238.0802	1278.7344
1288.0729	1309.0648	1341.3329
1354.2114	1378.1445	1385.8200
1392.7389	1411.9149	1471.4498
1501.1832	1507.4625	1519.4446
1566.9382	1597.5704	2991.4266
3025.9407	3030.0454	3042.5185
3073.1804	3077.1268	3083.3845
3090.1578	3116.0355	3190.5243

ROTATIONAL CONSTANTS (GHZ):            2.97569    1.58837    1.33456

\*\*\*\*\*

cyC6OO\_ax->HO2 + cyC6H10



```
C -0.3786255818 0.3792833826 1.0518138441
C 0.461019351 1.4689582127 0.4522709147
C 1.3334359623 0.9692170487 -0.7061427208
C 2.0444775626 -0.3313770023 -0.3097095253
C 1.0339094447 -1.4552270729 -0.0289415282
C -0.1776341718 -0.9797512179 0.7931753175
H 1.1068586724 1.8598288918 1.2561516432
H 2.6453903898 -0.1454093916 0.5911442227
H 1.5278590861 -2.2753212862 0.5040237605
H -1.2182649465 -1.0693181668 -0.030230204
H -0.1743740284 2.3070558997 0.1454068148
H -0.526007747 -1.6665166994 1.5674674537
H 0.6949577832 -1.8796175444 -0.9832937862
H 2.7428180337 -0.6460860231 -1.0931159051
H 2.0595682392 1.7407106349 -0.9840860739
H 0.7032454238 0.7929510646 -1.5872039274
H -1.0445542746 0.6668776894 1.8606485203
O -2.1089939162 0.60946099 -0.3539448476
O -2.1931300881 -0.6084328868 -0.7412689438
```

Frequencies:

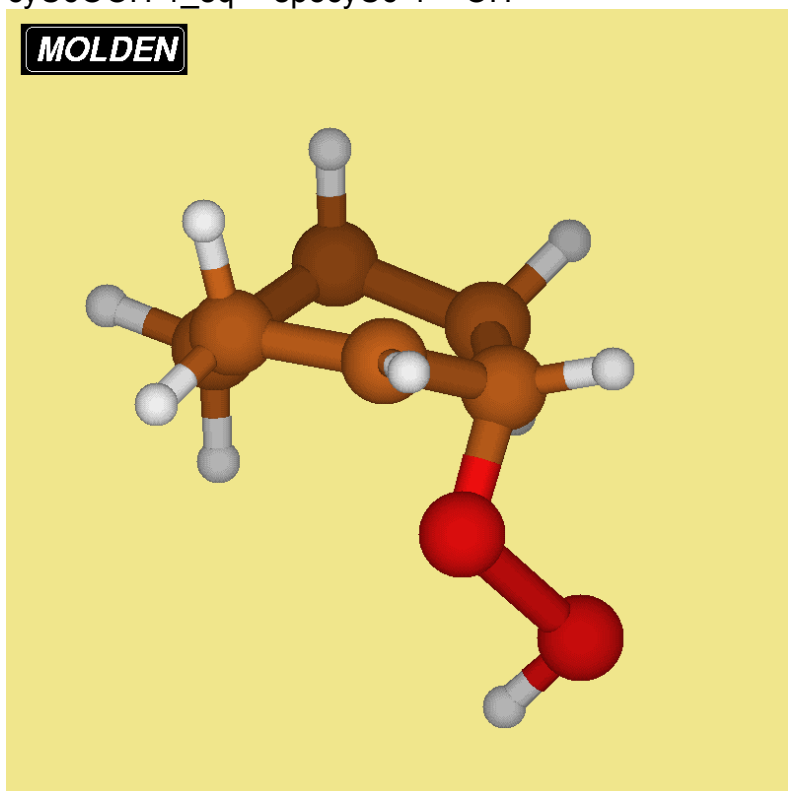
-992.0019	83.4970	121.8014
195.9023	218.6134	312.4966
395.9936	443.1155	469.6371
542.8538	645.7381	711.6122

796.9223	819.9133	829.4331
887.9885	911.2930	946.3885
973.1776	1029.2555	1054.1940
1077.1453	1107.9563	1152.7073
1185.3114	1238.1587	1278.7482
1287.6442	1308.9936	1341.3897
1354.1300	1378.2122	1385.8386
1392.6572	1411.7542	1471.5522
1501.1602	1507.4866	1519.4211
1567.1322	1597.7582	2990.9672
3025.7060	3029.9397	3042.5845
3073.4022	3077.3605	3083.3779
3090.3056	3116.0218	3190.3159

Rotational constants (GHZ):      2.97506    1.58972    1.33575

\*\*\*\*\*

cyC6OOH-1\_eq-> epocyC6-1 + OH



C	0.86384	1.258	2.09849
C	1.31465	0.478	3.28043
O	0.75116	2.3191	3.02134
C	1.87457	1.49977	0.96909
C	2.75056	0.41125	3.67407



C	3.32097	1.09372	1.31765
C	3.64452	1.30655	2.80189
H	-0.11923	0.95768	1.71432
H	0.56066	0.0206	3.91295
H	1.54648	0.968	0.06899
H	1.80582	2.56923	0.74693
H	2.86353	0.64614	4.74111
H	3.07619	-0.63982	3.57359
H	3.47429	0.03201	1.07873
H	4.02262	1.65216	0.68848
H	3.47609	2.35423	3.07366
H	4.6972	1.08103	3.00387
O	0.11237	3.6966	2.18188
H	0.63278	4.32089	2.71382

Frequencies:

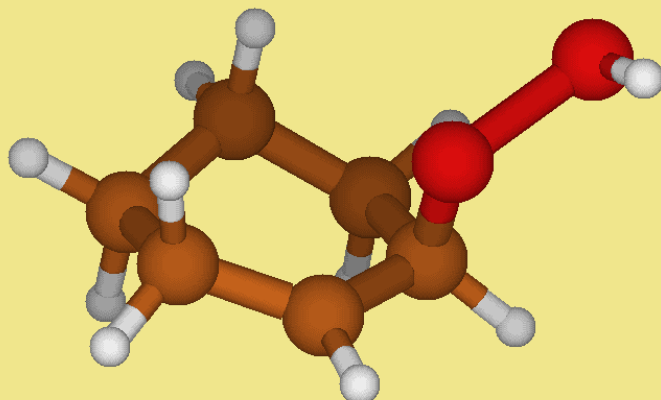
-693.6315	69.5893	121.3087
136.7123	166.6273	260.3624
295.0936	377.9392	408.2513
456.6642	524.7614	653.2123
700.3883	802.3128	819.3739
858.0766	874.8982	897.0100
962.2706	997.0796	1018.4222
1055.0112	1062.8670	1087.5528
1141.3611	1179.1512	1205.7483
1263.8983	1295.1480	1309.5954
1357.6363	1368.0686	1374.4998
1395.5843	1414.2648	1425.2189
1467.7106	1497.2633	1504.2962
1516.1268	2963.6065	3023.2715
3036.6086	3039.3381	3056.6549
3060.7714	3079.0738	3100.7242
3109.5454	3208.9526	3785.4467

ROTATIONAL CONSTANTS (GHZ)      3.08976    1.61892    1.36694

\*\*\*\*\*

cyC6OOH-1\_ax-> epocyC6-1 + OH

**MOLDEN**



```
C 0.310092503 -1.3380483121 0.4936246707
C -0.6081073813 -0.2134190251 0.8123234799
C -0.0149331423 1.1899777935 0.7669783133
C 0.9992119908 1.3453188438 -0.3736845179
C 2.0992602461 0.2788473599 -0.2769504175
C 1.5206431838 -1.1467025786 -0.3606680725
O -1.2643244959 -0.6086197775 -0.3651097233
O -2.7212880045 0.3600158919 -0.5220403403
H 0.4688174611 1.3919769861 1.7329841966
H 2.6306723456 0.3958873907 0.6772937856
H 2.2765420495 -1.894571326 -0.0862973168
H -3.2847600971 -0.4272819161 -0.6025461126
H -0.8416523132 1.8988344109 0.6600003855
H 0.0109373966 -2.3389167179 0.7871554504
H 1.2495548689 -1.3743698658 -1.4034752886
H 2.8444561471 0.4142784846 -1.0684884812
H 1.4426003704 2.3467193389 -0.3450205342
H 0.4750151644 1.2523019492 -1.3315938682
H -1.2242877908 -0.3718721383 1.7074475578
```

Frequencies:

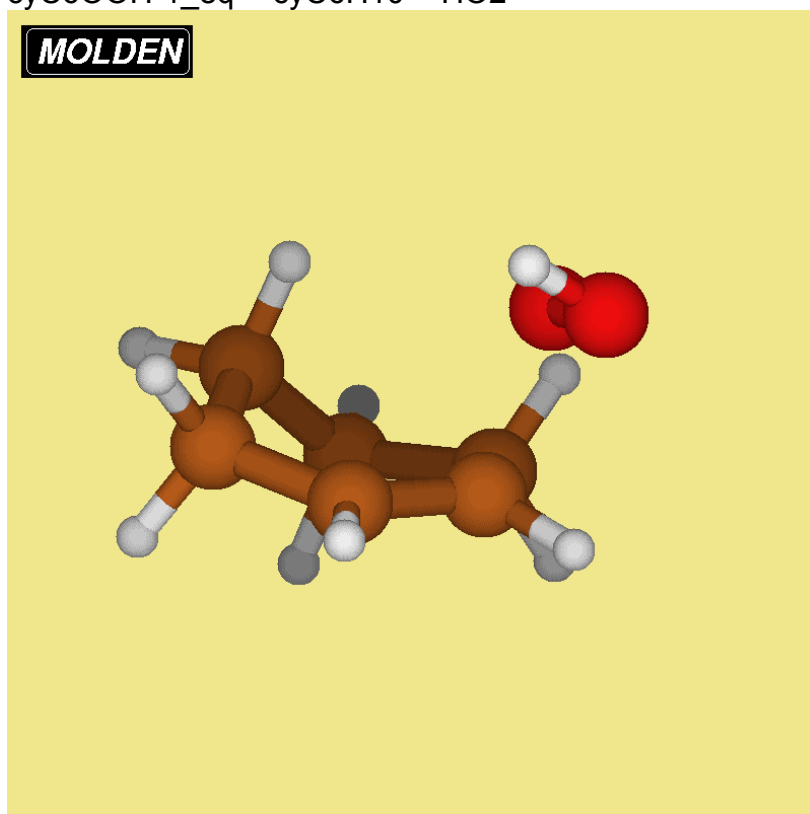
-702.4614	76.1926	142.6918
149.4278	173.6473	260.9143

296.9663	376.1535	403.9782
469.7754	521.0809	663.8551
689.8856	795.3067	812.1885
864.6385	874.8453	906.3339
938.6072	992.4143	1015.4335
1055.6193	1064.3394	1085.1268
1139.8813	1169.1872	1210.1442
1262.0436	1289.0089	1308.3627
1358.2097	1371.7032	1383.8678
1394.7362	1410.6459	1428.9532
1467.2519	1486.9063	1504.0657
1514.0377	3001.7584	3024.6032
3028.8333	3038.2772	3050.5225
3053.1030	3082.6714	3097.2822
3106.4346	3210.1891	3782.9802

Rotational constants (GHZ):      3.34336    1.57431    1.29789

\*\*\*\*\*

cyC6OOH-1\_eq-> cyC6H10 + HO2



C -0.2503033687 0.6694777902 -0.7061636481  
C -0.0681254819 1.1673083046 0.580059257  
C 0.87620193 0.546352511 1.5669307227  
C 1.4994174094 -0.7517397225 1.0325791948

C 1.9716330566 -0.5532137013 -0.4128353327  
C 0.7831703974 -0.2439470663 -1.3402869208  
H -0.711165604 1.9735825348 0.9265522051  
H 0.7466855203 -1.5491650706 1.0596224221  
H 2.5027208246 -1.4401429275 -0.7751777334  
H 1.1373500541 0.2164547146 -2.2707185655  
H 0.2765719842 -1.1709958073 -1.6350671531  
H 2.6914237707 0.2760355923 -0.4415635017  
H 2.3286342605 -1.0650404858 1.6762881626  
H 0.356488441 0.3643817805 2.5186150081  
O -1.6227525958 -0.6309423513 -0.4522941075  
O -2.8711761396 -0.0016997456 -0.3481210707  
H -0.8559560587 1.2580050476 -1.3885983261  
H 1.671960007 1.2704710131 1.8102609727  
H -3.0652469734 -0.0778783112 0.6014082964

Frequencies:

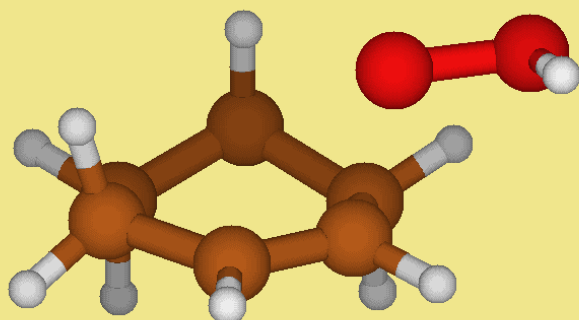
-484.8173	55.1957	88.5358
142.9092	196.3879	288.9233
330.0283	354.9742	406.2701
461.1708	499.4077	673.5712
721.4578	811.3165	825.0096
885.3296	893.4500	914.7992
960.5054	1012.6966	1050.3123
1058.6619	1070.5934	1084.5207
1156.1922	1165.1835	1227.9612
1266.8476	1297.5477	1354.0962
1371.4985	1377.5303	1378.8857
1393.5128	1424.4560	1470.9891
1488.2066	1506.7345	1517.3187
1521.3122	2980.0992	3024.6183
3029.6400	3041.9837	3047.2953
3073.0841	3085.9775	3092.0662
3165.1811	3190.1879	3713.4797

Rotational constants (GHZ): 3.28044 1.41320 1.21909

\*\*\*\*\*

cyC6OOH-1\_ax-> cyC6H10 + HO2

**MOLDEN**



```
C 0.4847425763 -1.3508959088 0.4678010307
C -0.420117524 -0.3585546386 0.8184229914
C -0.0291125284 1.0990303608 0.7635372302
C 0.9954129344 1.3665114624 -0.3461871938
C 2.1764310974 0.3902287057 -0.2493679106
C 1.7040653134 -1.070587665 -0.359586599
O -1.6550181781 -0.4127310599 -0.6907943743
O -2.8420758378 0.2015738248 -0.2654948487
H 0.3949444329 1.3784413517 1.7403722168
H 2.6842304196 0.5320541621 0.7141945636
H 2.5114451879 -1.7625316323 -0.0865603834
H -3.416632273 -0.5584738607 -0.0668623837
H -0.9294217826 1.7057131894 0.6280274725
H 0.2339648292 -2.3891110424 0.672816458
H 1.4679445943 -1.300961392 -1.412835254
H 2.9180801296 0.6001949967 -1.0282340116
H 1.3500708071 2.4018526227 -0.2898167677
H 0.496216581 1.247368634 -1.3149730349
H -1.2026220127 -0.6196830486 1.5264676144
```

Frequencies:

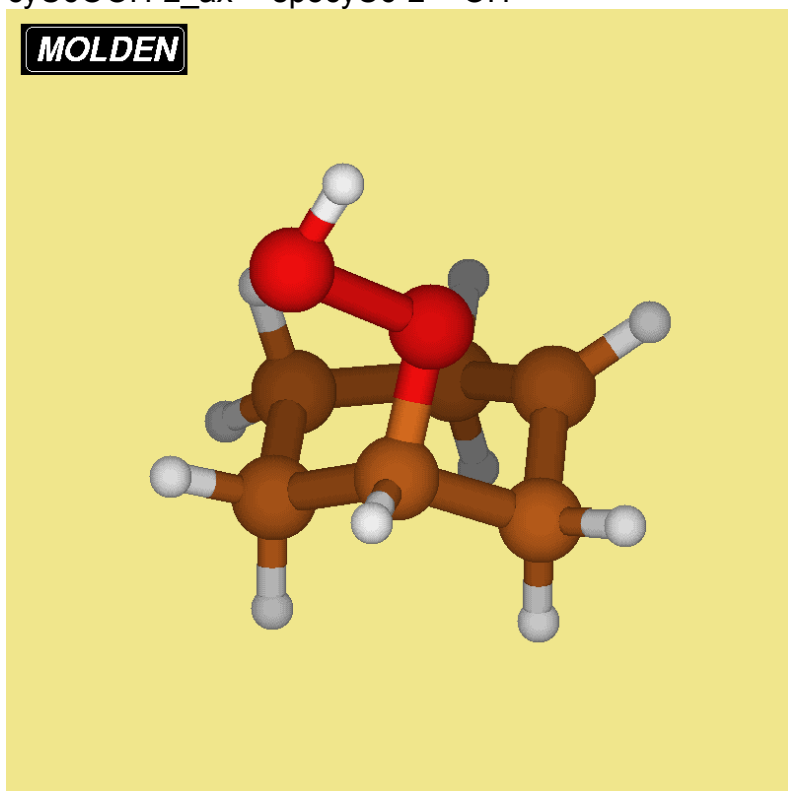
-503.3161	31.5022	100.6156
141.4081	231.1525	282.4216
310.5796	386.7336	429.2666

462.7929	506.4031	664.0350
728.6067	816.9875	827.3894
884.2031	900.9457	920.0201
943.5496	1014.9716	1030.3689
1047.1495	1068.6759	1087.7114
1150.1769	1158.3502	1230.9718
1266.4042	1298.8985	1356.2961
1360.8779	1374.3469	1386.0730
1394.4328	1425.3359	1471.4684
1491.2201	1504.3778	1514.3455
1526.3213	2975.5679	3007.8251
3029.1622	3047.9603	3049.8654
3079.1160	3093.0087	3099.1484
3162.5565	3179.7626	3695.4155

Rotational constants (GHZ):        3.48078    1.38928    1.18777

\*\*\*\*\*

cyC6OOH-2\_ax-> epocyC6-2 + OH



C	0.17913	0.39135	0.07406
C	-0.06109	-0.46062	1.32331
C	1.07065	0.14437	2.11016
C	2.45207	-0.22169	1.65823
C	2.6757	0.12808	0.1634

C	1.41584	-0.09482	-0.69513
H	0.03421	-1.54397	1.15903
H	2.57739	-1.30918	1.80377
H	3.52563	-0.43625	-0.23465
H	1.51179	0.46197	-1.6317
H	-1.03433	-0.24755	1.7707
H	1.28284	-1.15355	-0.95561
H	2.92824	1.18943	0.10535
H	3.21401	0.26372	2.27636
H	0.91279	0.54305	3.10736
H	-0.68532	0.5584	-0.57423
O	0.50285	1.60468	0.7971
O	0.4594	2.75976	-0.47709
H	0.34611	3.50589	0.13283

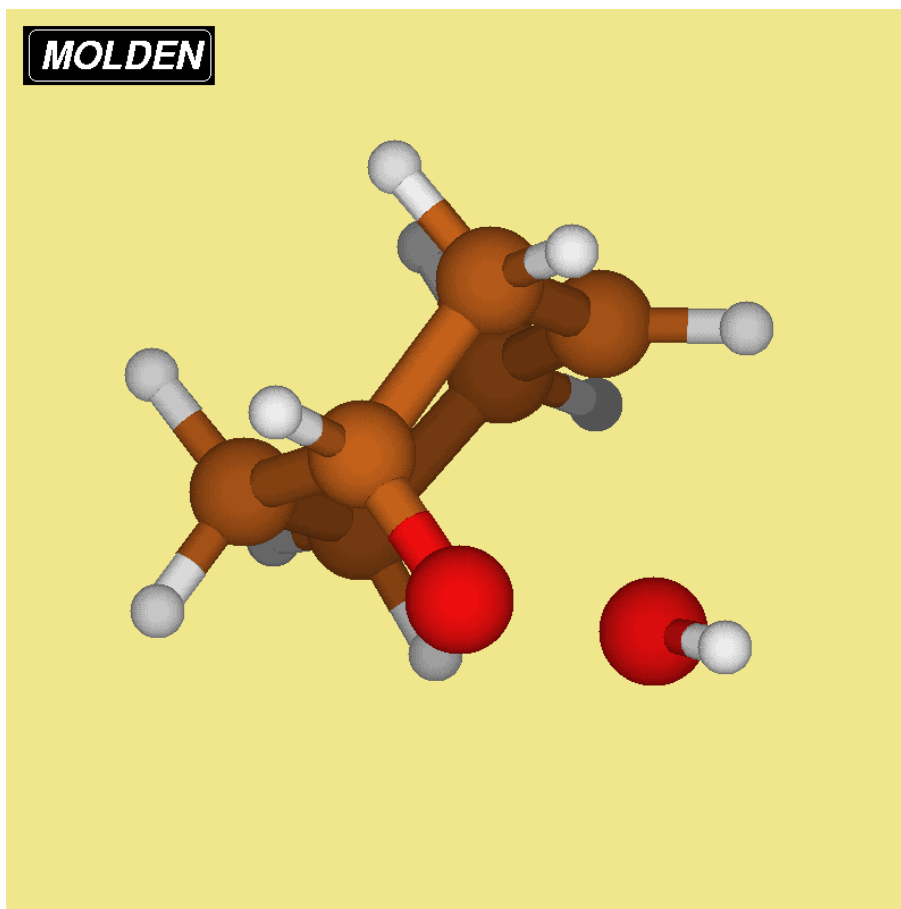
Frequencies:

-732.5338	106.0201	142.0395
192.0875	229.2360	295.1476
347.5351	392.3747	417.5228
519.2153	560.0182	666.3132
739.3788	822.0190	854.9067
864.7194	881.5207	928.0563
954.5570	1015.8579	1021.7335
1044.2776	1067.5767	1104.3339
1113.2657	1134.5889	1190.3526
1220.8446	1261.7197	1297.1617
1306.8687	1348.1193	1348.8300
1366.3819	1391.3956	1401.5528
1484.8750	1491.6460	1498.1954
1510.5381	2965.7309	3012.0886
3036.5379	3065.5239	3086.3119
3094.8009	3104.2265	3120.6705
3123.9972	3199.8785	3794.9387

ROTATIONAL CONSTANTS (GHZ)      2.87608    1.87338    1.63220

\*\*\*\*\*

cyC6OOH-2\_ax -> cyC6O\_OH-2\_ax; original basis?

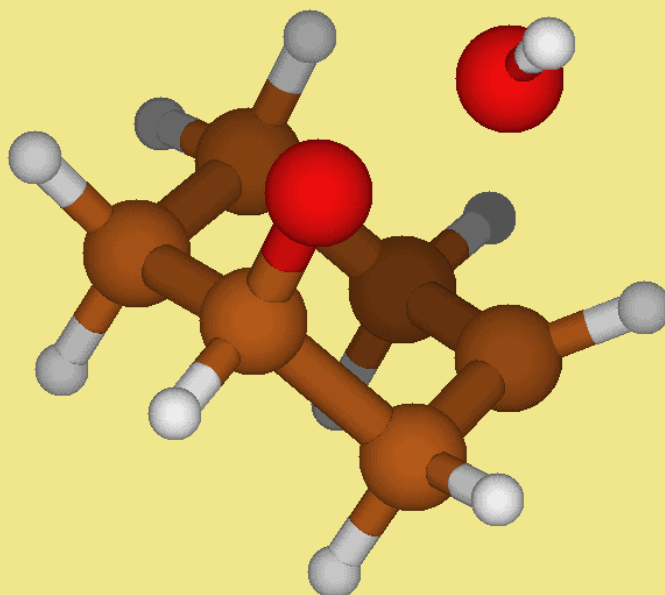


C	-0.853839	0.395123	0.760294
C	0.235530	1.468955	0.574125
C	1.303895	1.044946	-0.445303
C	1.903997	-0.346692	-0.098613
C	0.824182	-1.328049	0.209546
C	-0.152387	-0.974288	1.229624
H	0.702470	1.672130	1.549007
H	2.545525	-0.230209	0.792307
H	0.750955	-2.257094	-0.339621
H	-0.917374	-1.737285	1.387775
H	-0.245759	2.396464	0.246236
H	0.324639	-0.733791	2.189989
H	-1.569466	-1.278877	-1.644990
H	2.545659	-0.699978	-0.910797
H	2.109479	1.787173	-0.485733
H	0.846700	0.989832	-1.435537
H	-1.524811	0.659729	1.595522
O	-1.670988	0.204515	-0.307789
O	-0.764839	-0.747201	-1.544279

cyC6OOH-2\_ax -> cyC6O\_OH-2\_ax; larger basis ?



**MOLDEN**



C	0.725646	0.761376	0.678975
C	0.107180	-0.553970	1.449843
C	-0.664885	-1.301505	0.483750
C	-1.799801	-0.619588	-0.190388
C	-1.267182	0.643191	-0.933677
C	-0.431696	1.521556	0.006358
H	-0.518500	-0.113332	2.234052
H	-2.535985	-0.287271	0.557177
H	-2.117133	1.208288	-1.328777
H	-0.006283	2.363679	-0.546433
H	0.934889	-1.107189	1.890503
H	-1.074512	1.940323	0.792385
H	-0.650836	0.326665	-1.776631
H	-2.312240	-1.283814	-0.888923
H	-0.289575	-2.238557	0.098378
H	1.148915	1.339053	1.515766
O	1.780404	0.465975	-0.102750
O	1.357134	-0.936021	-1.177933
H	2.305391	-1.093832	-1.271199

Frequencies:

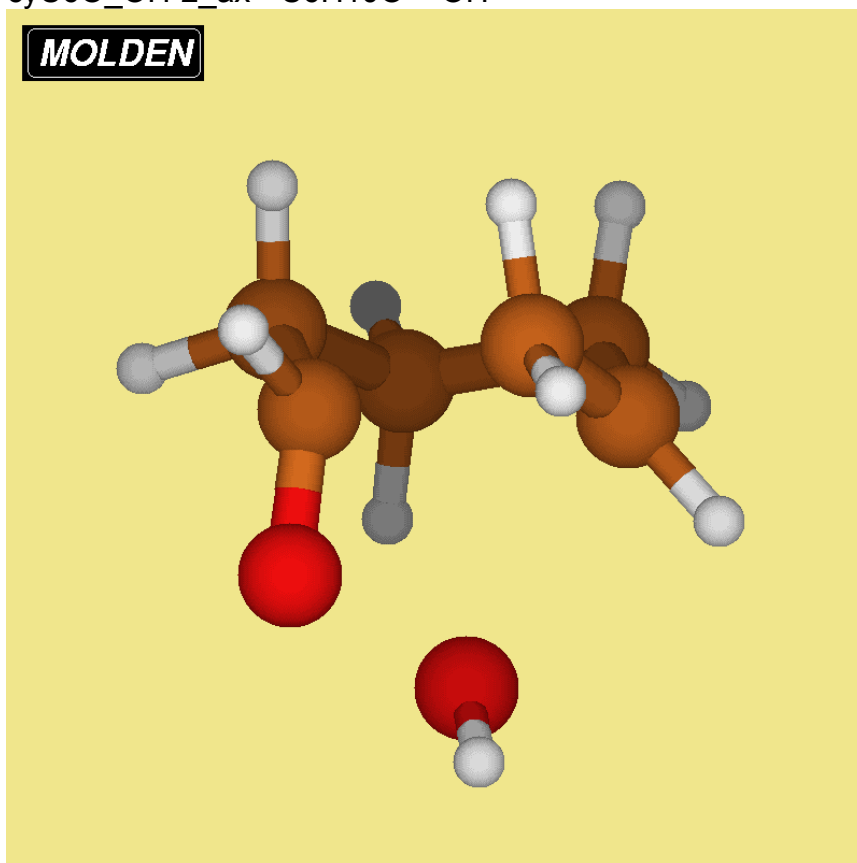
-788.7080	97.7476	117.7150
-----------	---------	----------

225.3989	240.3425	258.4034
346.1137	390.2868	407.0348
465.6291	495.7113	571.5817
711.5625	728.4984	794.4865
853.5101	874.5102	890.5188
907.7530	964.1102	993.0333
1006.5878	1049.2815	1077.0969
1127.2493	1166.1421	1176.6066
1211.1108	1248.2799	1266.0404
1290.1279	1320.5168	1331.2193
1358.0656	1379.6295	1421.0470
1475.4640	1482.5681	1491.3936
1496.2405	2967.0947	2971.8310
3001.6143	3022.7703	3037.6437
3069.0827	3083.4587	3104.8159
3127.1781	3217.8962	3821.7067

Rotational constants (GHZ):      2.60421    1.91095    1.76745

\*\*\*\*\*

cyC6O\_OH-2\_ax->C6H10O + OH



C	-0.94761	0.44645	0.75011
C	0.20247	1.45485	0.53219

C	1.29381	1.02092	-0.44956
C	1.88875	-0.37539	-0.08411
C	0.78248	-1.33169	0.20564
C	-0.08359	-1.05419	1.27359
H	0.6428	1.68574	1.51258
H	2.5073	-0.26369	0.81799
H	0.64335	-2.19908	-0.42573
H	-0.85167	-1.78959	1.50135
H	-0.26863	2.37474	0.16616
H	0.39394	-0.63889	2.16116
H	-1.42997	-1.22457	-1.70575
H	2.53285	-0.73322	-0.89099
H	2.1096	1.75265	-0.44925
H	0.87761	0.96832	-1.45516
H	-1.46764	0.66095	1.70524
O	-1.77906	0.17825	-0.20296
O	-0.65323	-0.64717	-1.64074

Frequencies:

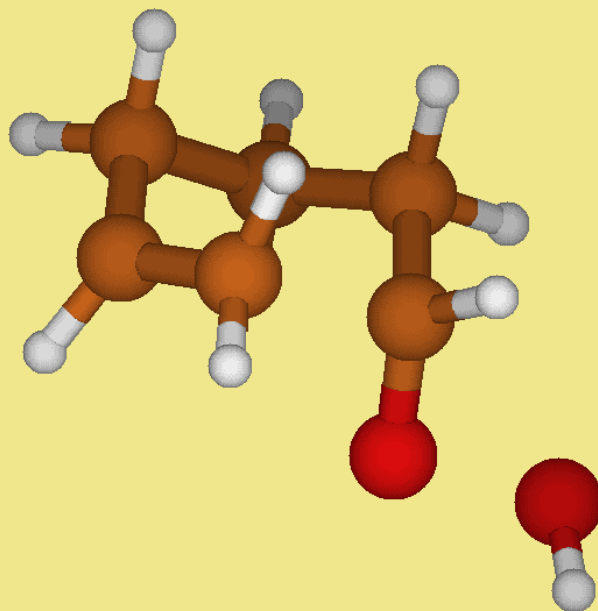
-480.6710	120.1359	155.7839
251.1412	262.7297	352.0248
404.0711	429.6901	449.0150
475.6058	504.3784	557.0899
655.3872	697.6693	746.7217
802.3526	858.9202	881.6834
899.0375	929.6719	985.0895
999.2822	1047.1262	1050.7381
1098.1360	1152.9432	1187.5354
1227.3014	1252.6280	1287.7486
1325.6425	1329.8949	1363.4910
1383.7645	1426.2357	1461.5589
1484.2358	1495.7678	1509.9537
1551.1118	2908.7899	3020.7452
3020.9081	3061.6757	3081.3758
3113.3053	3115.4390	3159.8232
3197.1841	3248.4445	3799.2402

Rotational constants (GHZ):        2.49705    1.97683    1.84821

\*\*\*\*\*

cyC6OOH-2\_ax -> >C6H10O + OH; external

**MOLDEN**



```
C 0.0621777571 0.4088429374 -0.1913720062
C 0.0169302395 -0.2294300794 1.5669805388
C 1.2423391348 0.1251759921 2.1625152868
C 2.5164898893 -0.3429435936 1.5472430509
C 2.6121481232 0.2937799995 0.1255854872
C 1.4048831883 -0.0921805541 -0.7296348849
H -0.091618728 -1.2726168074 1.2636112501
H 2.524339291 -1.436103097 1.4358533233
H 3.540973502 -0.0358525828 -0.3531470761
H 1.492175797 0.3509602227 -1.7286758296
H -0.8939703856 0.1856252127 1.9910248262
H 1.3574090245 -1.1822863577 -0.8550630618
H 2.6556500591 1.3846210174 0.2118519691
H 3.3859069749 -0.0621010327 2.1491667967
H 1.2785176272 1.0069756379 2.7986931493
H -0.7924592513 -0.1526970364 -0.611399877
O -0.1125918902 1.6934360161 -0.0597976299
O -0.0305616707 2.3880668492 -1.7613844865
H -0.8703996822 2.847783256 -1.5972408262
*****
```

cyC6OOH-3\_eq-> epocyC6-3 + OH

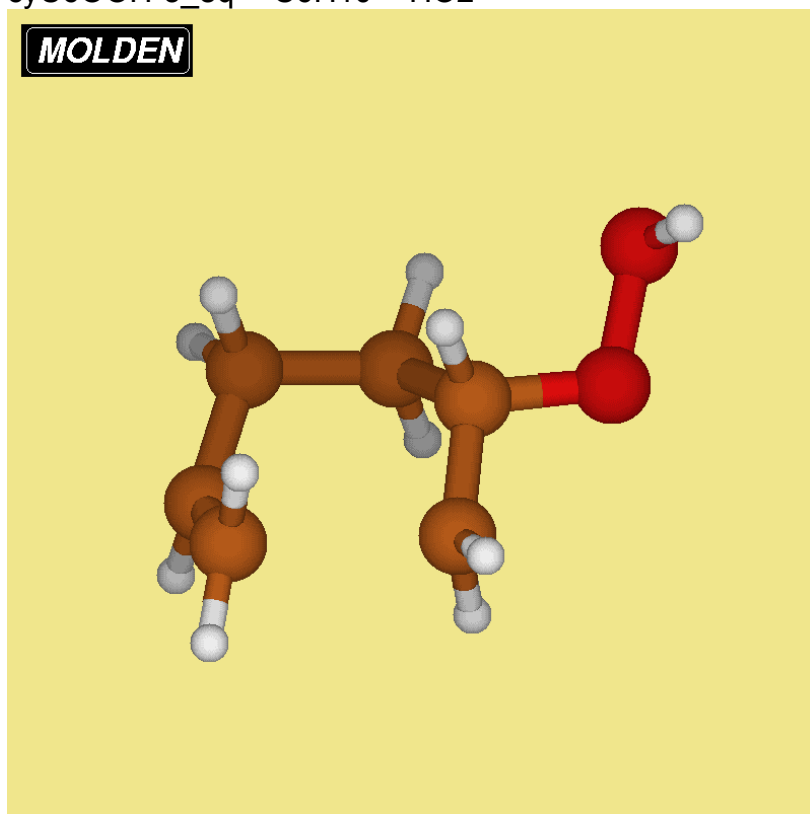


99.3929	200.9739	287.3218
318.3224	383.5289	401.1855
548.1758	572.7482	669.9623
787.5358	808.1067	833.0843
854.2683	889.4013	902.1573
930.8014	981.6060	1028.8123
1045.4342	1098.7953	1101.3527
1118.3423	1157.7859	1211.4047
1214.1592	1252.5935	1274.6714
1319.9352	1328.1979	1340.3873
1344.1200	1370.0463	1393.0234
1480.1375	1489.6030	1501.2281
1514.5222	2982.0719	2990.4740
3056.6465	3062.1167	3098.2073
3099.0433	3116.6599	3118.5616
3123.7751	3205.6773	3787.5264

ROTATIONAL CONSTANTS (GHZ)      2.93274    1.77397    1.59030

\*\*\*\*\*

cyC6OOH-3\_eq-> C6H10 + HO2



C -0.0112894239 0.0345395374 -0.0248239996  
C -0.0867384569 1.5619650803 0.1066751671  
C 0.180205292 2.0567802822 1.5515402276

C -0.8409779547 1.4752133885 2.4871139106  
C -0.7891900215 0.1657473719 2.8478778592  
C -1.096161164 -0.7125863734 0.6887838977  
H -1.0786135263 1.8912369121 -0.2270202267  
H -1.5913673471 -0.2989139095 3.4134518359  
H -0.9506724128 -1.7745229896 0.8662049046  
H 0.6472176301 1.9996521036 -0.5760994912  
H -2.1205436818 -0.4031987813 0.5038068993  
H 0.1512846318 -0.3783623144 2.8320599826  
H -1.7623386997 2.0345988056 2.6413315202  
H 0.1631850677 3.1515609841 1.5685410972  
O -0.1558401087 -0.3636931202 -1.4127747236  
O 1.0140714822 0.1304360405 -2.148642201  
H 0.9756929925 -0.3139631616 0.3176324126  
H 1.1908798807 1.7480645433 1.8511764515  
H 1.4608638204 -0.7136333995 -2.3236595238

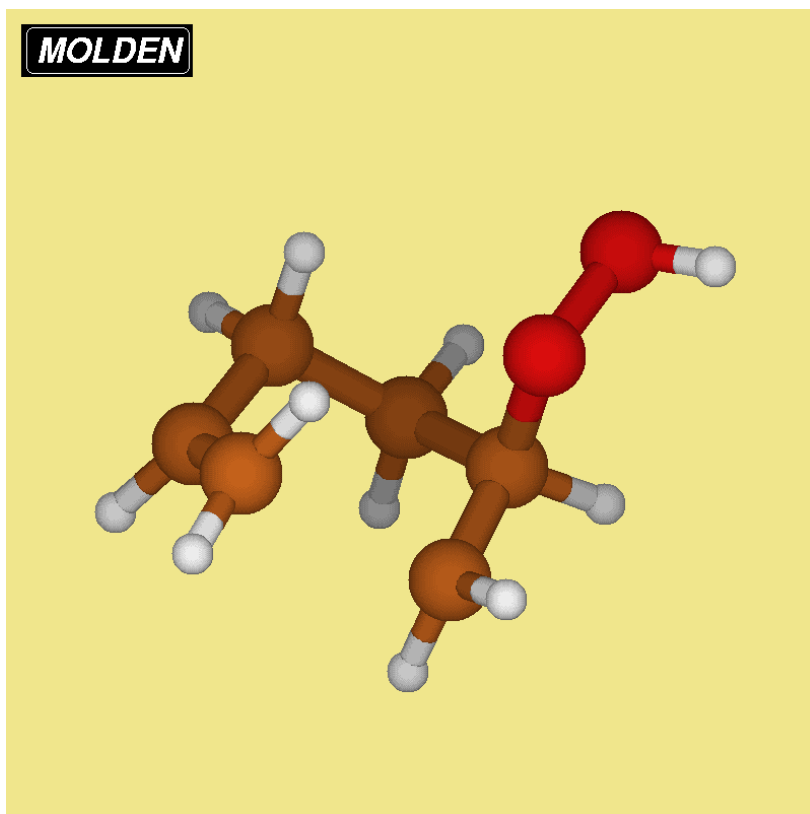
Frequencies:

-387.8978	85.3809	139.4633
195.4549	216.6609	256.4260
296.8283	350.9335	405.6912
433.3988	484.1116	515.1977
538.2764	697.2121	760.1860
816.5756	858.3001	866.7988
921.4335	934.6034	949.5731
972.7391	987.6101	1005.7696
1033.0012	1134.3682	1170.0327
1237.5277	1243.1789	1295.8839
1327.4454	1336.1950	1341.8478
1364.2623	1403.1337	1446.9286
1476.0587	1502.0426	1510.0157
1608.9117	2994.7680	3031.7010
3050.8423	3088.7780	3113.2718
3144.7033	3149.4051	3161.5515
3235.0050	3244.1417	3757.1188

ROTATIONAL CONSTANTS (GHZ)      3.91347    1.26144    1.03400

\*\*\*\*\*

cyC6OOH-3\_ax-> C6H10 + HO2



```
C 0.3292089568 -1.5092600153 0.7983766661
C -0.6671571606 -0.3905371169 0.7348738296
C -0.0796377307 1.0242221673 0.9026348433
C 0.8919145608 1.4338351398 -0.2335922549
C 2.0354101675 0.4641189642 -0.318724709
C 1.8485500614 -0.7807189778 -0.8331195609
O -1.3211295034 -0.5505638397 -0.541634177
O -2.4544366397 0.3618204322 -0.5782894841
H 0.4324199872 1.0641472958 1.8728218328
H 2.6306856756 -1.5332809459 -0.7884112297
H 0.0013986719 -2.4816082089 0.4403154345
H -0.9088378585 1.737079982 0.9470781959
H 0.9903429852 -1.5193869712 1.6586574572
H 1.0371868013 -0.9749196832 -1.5273395769
H 2.9238983035 0.6709560589 0.2765712066
H 1.2422583618 2.4553632036 -0.0488904349
H -1.4397690849 -0.5283848292 1.5160248635
H -3.1839616573 -0.2764116218 -0.51694549
H 0.3291738272 1.4464320122 -1.173185856
```

Frequencies:

-416.5159	85.2228	119.9305
188.8429	225.0641	277.3294
305.5579	324.8532	392.5782



442.9122	503.3146	541.0182
617.4048	701.8407	722.9887
810.5467	854.0868	892.7860
930.4404	941.3084	953.3383
957.5353	980.1361	1010.3408
1054.3327	1137.9259	1151.5234
1222.5402	1244.5287	1297.4343
1324.5728	1333.9031	1359.1095
1375.1082	1384.4009	1443.4747
1456.1587	1492.0389	1506.6002
1604.4659	2912.7176	3043.5602
3052.6720	3096.6386	3103.2943
3145.8365	3149.8235	3158.8969
3242.4292	3247.1197	3752.3669

Rotational constants (GHZ):      3.03000    1.56868    1.35762

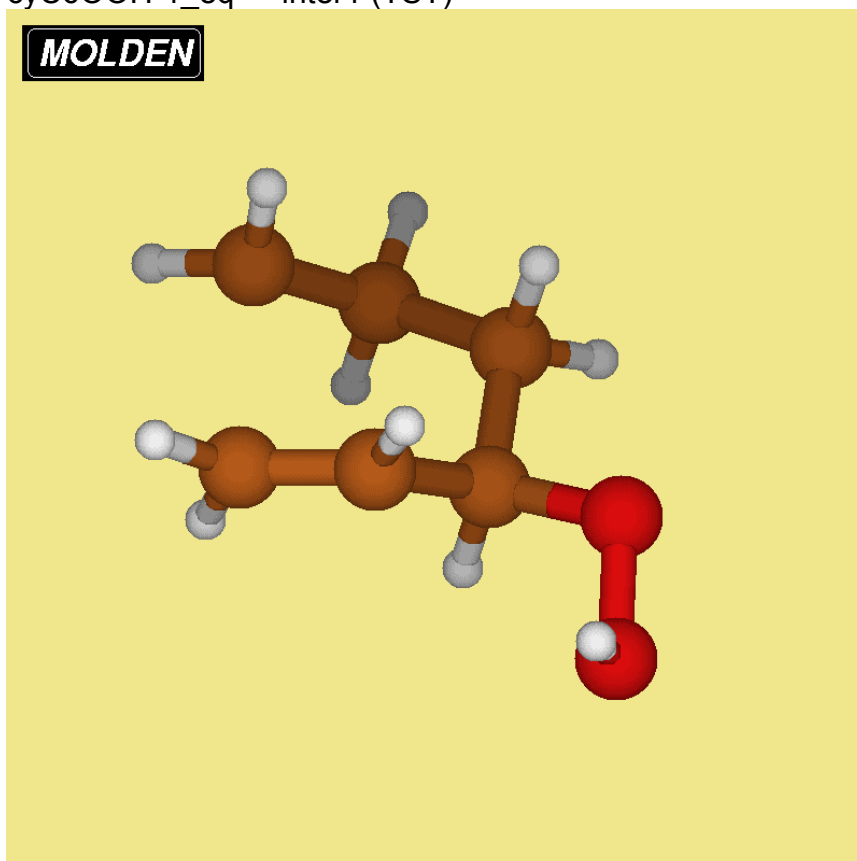
\*\*\*\*\*

beta decomposition paths: involve the formation of an intermediate state

\*\*\*\*\*

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cyC6OOH-1\_eq -> inter1 (TST)



C -0.4158386889 0.2799052341 -0.4425622828  
C -0.4966689627 0.1817486603 1.0528108416  
C 0.5288023801 0.6287960163 1.8216713876  
C 2.1580248338 -0.8618551002 1.0065185466  
C 1.9745326374 -0.6559391411 -0.4712942997  
C 0.5287879088 -0.8116154462 -0.989433176  
H -1.2164172906 -0.5332253244 1.4506080657  
H 1.7752752999 -1.7811429004 1.4430407829  
H 2.6006342681 -1.3770088993 -1.0243477961  
H 0.5185495154 -0.7587454289 -2.0835373954  
H 0.1328043275 -1.7957642805 -0.7097290203  
H 2.3547163814 0.3343267839 -0.7581755069  
H 3.0650968731 -0.4783030583 1.4675415034  
H 0.5625846291 0.4361635183 2.8894941238  
O -1.6700608486 0.0441602228 -1.0878806194  
O -2.5243972974 1.1888118588 -0.8101664607  
H -0.0382784807 1.2662072087 -0.7479151622  
H 1.1896602538 1.4132471699 1.4637423593  
H -3.0548012592 0.8442272193 -0.072611417

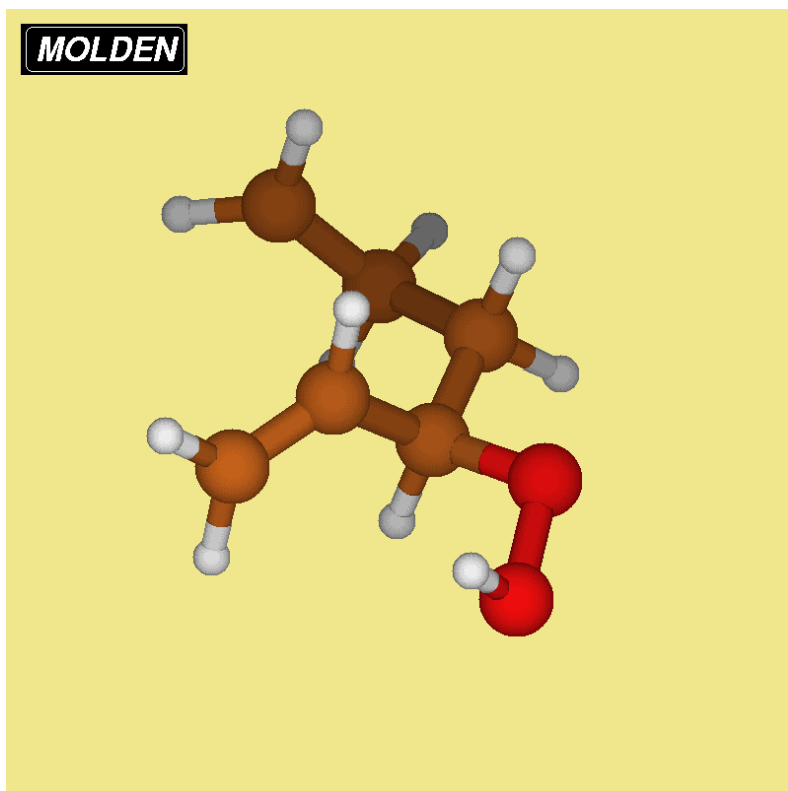
Frequencies:

-412.4586	91.2891	120.9012
178.1603	218.6955	243.8572
307.2765	310.4094	375.1582
450.4740	472.4911	511.4788
569.5160	677.2725	740.4207
827.2026	871.6593	890.4633
920.2664	931.0793	942.7569
972.9508	998.6641	1065.5784
1080.2117	1119.5080	1170.9932
1228.3543	1241.4142	1282.1517
1314.0158	1351.4529	1359.4791
1366.1512	1378.0628	1452.4145
1474.3322	1486.9496	1505.7786
1603.0847	2966.7859	3021.8930
3035.3978	3049.5016	3096.0989
3132.1926	3148.6961	3155.7302
3226.1102	3238.1436	3746.8344

Rotational constants (GHZ): 3.64047 1.33511 1.05324

\*\*\*\*\*

inter1: CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(OOH)CHCH<sub>2</sub>



```
C 0.2122574409 -0.1025538988 0.038970166
C 0.120940748 -0.2127263918 1.5391067403
C 0.1893109712 0.8300467502 2.3697360836
C 2.8734995551 -1.5923082457 1.0935843738
C 2.5371404238 -1.160817149 -0.2938821098
C 1.0329194168 -1.2057112381 -0.6377568938
H -0.0872426756 -1.2084799064 1.9293013094
H 2.4746573123 -2.5221671857 1.4881093151
H 3.0512510929 -1.8136009188 -1.0214207945
H 0.8971046196 -1.0968478981 -1.7189591584
H 0.617471845 -2.183620542 -0.3630445455
H 2.9255031338 -0.1521139222 -0.4819049453
H 3.6192794718 -1.0744880733 1.6853544393
H 0.0715276066 0.7171369255 3.4435655607
O -1.1080785895 -0.2426204927 -0.5313497757
O -1.8594017946 0.9562473223 -0.22429293
H 0.6012683417 0.8844722286 -0.243550981
H 0.3875527621 1.8340930859 2.0026825223
H -2.1429446821 0.7751485501 0.6897356236
```

Frequencies:

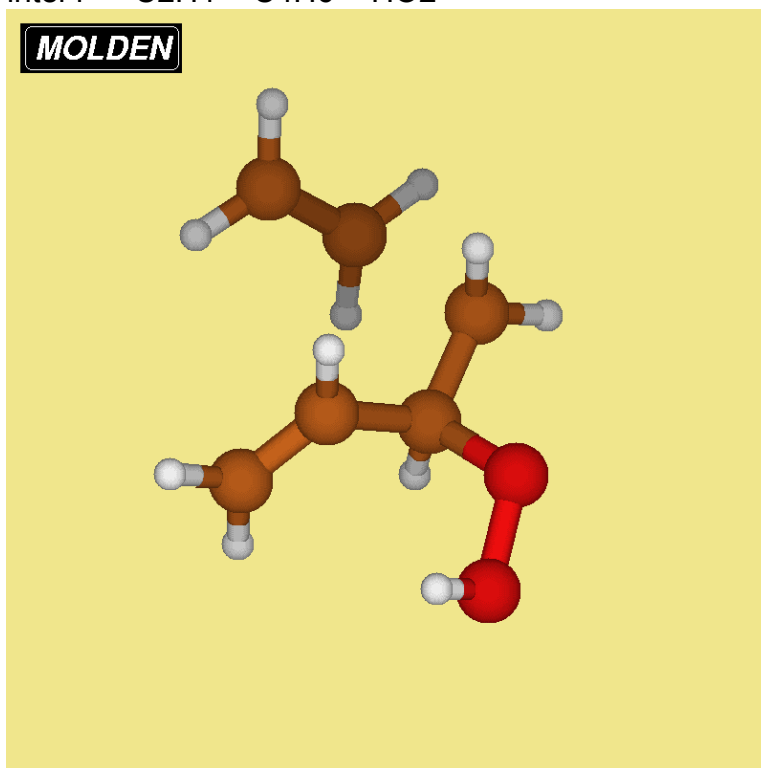
50.1080	85.3991	105.9627
131.8082	165.0357	190.9811
257.8850	276.1037	309.1159

365.9095	433.4350	453.2773
505.9366	509.9640	707.1351
806.7406	848.1931	910.6791
927.0488	950.0767	955.7534
1005.2337	1027.5065	1033.6464
1095.4805	1125.5953	1182.1782
1231.9923	1253.5407	1316.6627
1323.1807	1367.4103	1370.0088
1384.9663	1393.4639	1469.3643
1475.1066	1486.4674	1510.2541
1714.4519	2954.7331	3039.3516
3045.7556	3061.0132	3097.3720
3147.5402	3156.9712	3159.7050
3236.9012	3263.7539	3706.3561

Rotational constants (GHZ):      3.04011    1.33842    1.00504

\*\*\*\*\*

inter1 -> C2H4 + C4H6 + HO2



C	0.05093	-0.11709	-0.00633
C	0.00783	-0.21482	1.49587
C	0.19405	0.81931	2.31808
C	3.19226	-1.67919	1.08449
C	2.96699	-1.18884	-0.16223
C	0.6969	-1.28694	-0.67491

H	-0.24919	-1.19436	1.89845
H	3.36716	-2.73744	1.25487
H	3.14888	-1.8045	-1.03749
H	0.81507	-1.22355	-1.75284
H	0.47514	-2.27663	-0.2872
H	2.93092	-0.11787	-0.33669
H	3.13257	-1.04488	1.96282
H	0.11354	0.71651	3.39644
O	-1.31639	-0.09976	-0.52345
O	-1.89775	1.19519	-0.20464
H	0.51853	0.8261	-0.31567
H	0.44769	1.80616	1.93867
H	-2.18111	1.05169	0.71574

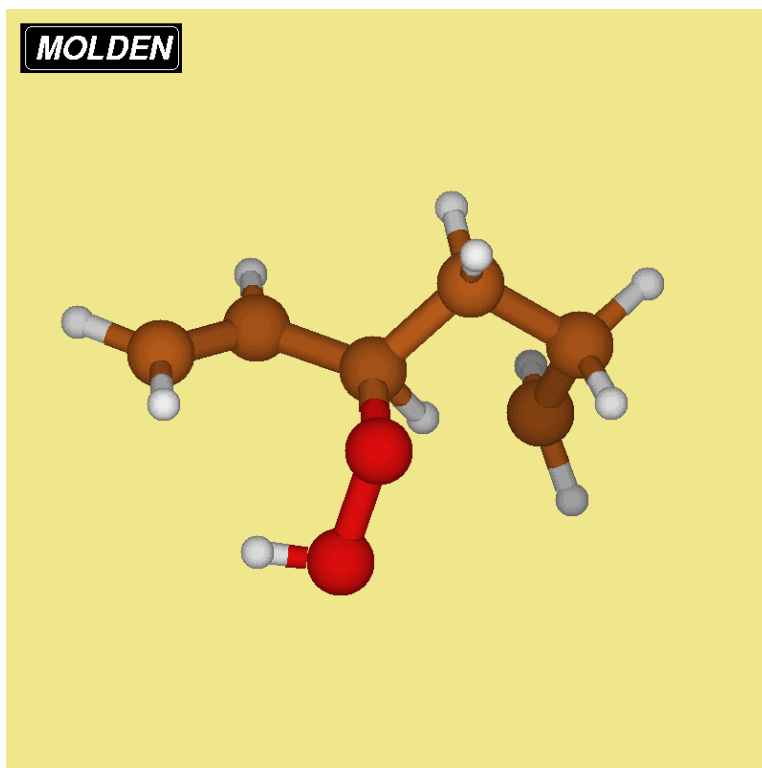
Frequencies:

-355.0916	33.9768	67.1899
81.5530	114.1080	161.9539
217.1348	243.4774	290.8695
336.4195	364.5774	384.1976
435.5252	525.3320	558.4195
713.5227	776.2261	825.8076
859.3038	872.5635	893.6409
919.4228	957.0070	974.3078
1000.9946	1024.3853	1032.1803
1139.0602	1206.0028	1243.8278
1311.5764	1316.4901	1321.7223
1360.6603	1374.2247	1471.5942
1476.9120	1480.8568	1600.6857
1719.1970	3045.0967	3145.5676
3147.2316	3153.4439	3158.1289
3162.4266	3232.7598	3236.4282
3246.2898	3258.3276	3712.5004

Rotational constants (GHZ): 3.06777 1.11320 0.88614

\*\*\*\*\*

inter1 -> Htrasp



```
C 0.5221233167 -0.389804071 0.6453701773
C -0.233379023 -0.4649972978 1.9093579677
C -1.3703377051 0.1964548078 2.1785083844
C 3.0118020727 -0.5899192902 0.2156160733
C 2.2208464118 -1.4089539694 -0.7872649903
C 0.8524311337 -1.6786999999 -0.1141900258
H 0.209060301 -1.101670311 2.6752079312
H 3.4867155964 -1.1363243686 1.0319112658
H 2.7221445443 -2.3424080173 -1.0693022648
H 0.0599694495 -1.9505674665 -0.8196087642
H 0.9355666023 -2.4931890622 0.6153493041
H 2.0647093468 -0.8287256647 -1.7011322804
H 3.5879755793 0.2631564501 -0.1350353836
H -1.8582730751 0.1171490036 3.1439512167
O 0.0457615004 0.5603939985 -0.2789919577
O 0.4519965918 1.8956273051 0.1529323374
H 1.7845845392 -0.0955446276 0.8361155488
H -1.8702211376 0.7966395372 1.4225837419
H -0.2094590451 2.080473044 0.8426067184
```

Frequencies:

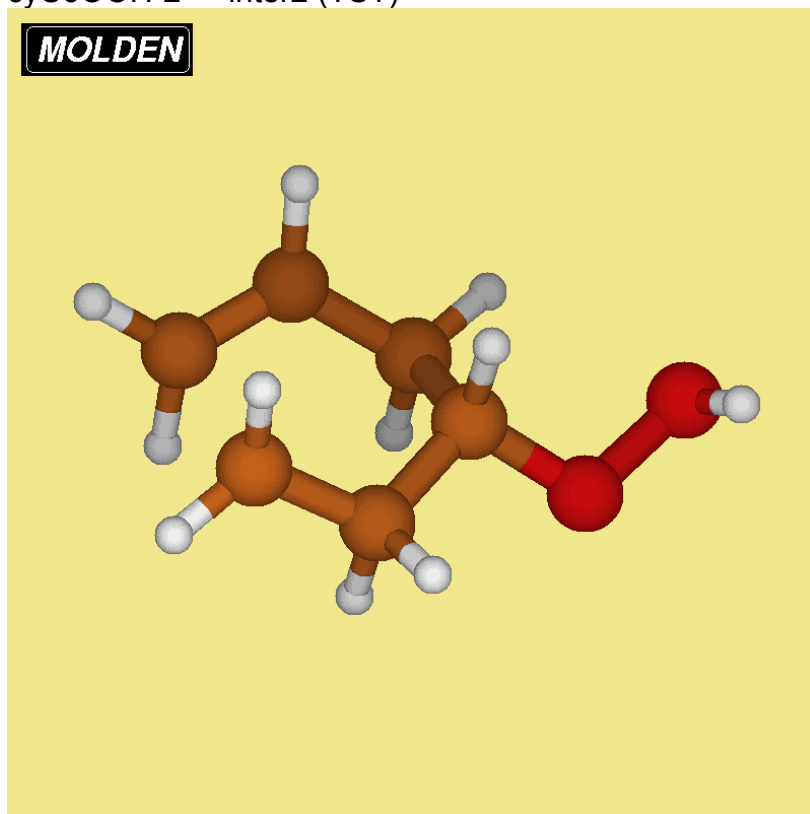
-1744.3182	94.2106	104.7935
163.5747	173.0359	219.7028
276.6183	296.7822	314.2311
400.4605	470.8687	511.3222

594.2408	637.8209	698.1185
807.4574	856.4910	888.3710
899.6778	911.9389	935.3171
989.7492	1001.5129	1020.1211
1048.0470	1071.6322	1136.3634
1205.4757	1220.5298	1261.7780
1318.1785	1333.4786	1348.8380
1378.6573	1410.9742	1454.2981
1468.2524	1488.2248	1507.0332
1621.5291	1665.6702	3050.3641
3056.5894	3097.6218	3109.5343
3116.3795	3150.1753	3158.0612
3210.4395	3246.0001	3720.9393

Rotational constants (GHZ):      2.95416    1.46648    1.20360

\*\*\*\*\*

cyC6OOH-2 -> inter2 (TST)



C	0.11937	0.28532	-0.09438
C	0.01445	-0.29707	1.33397
C	1.16936	0.19074	2.15938
C	2.41761	-0.31288	1.96948
C	2.66899	0.38273	-0.26212
C	1.39188	-0.15541	-0.84238

H	0.02269	-1.39076	1.24568
H	2.55827	-1.30808	1.55715
H	3.59502	-0.11095	-0.54564
H	1.27678	0.16885	-1.89052
H	-0.95015	-0.00395	1.75664
H	1.41707	-1.25253	-0.87192
H	2.74839	1.4565	-0.11413
H	3.28249	0.11527	2.46783
H	1.04755	1.12738	2.7006
O	-0.95247	-0.17384	-0.92762
O	-2.19548	0.36478	-0.39311
H	-2.40263	1.01699	-1.08241
H	0.08291	1.38454	-0.04666

Frequencies:

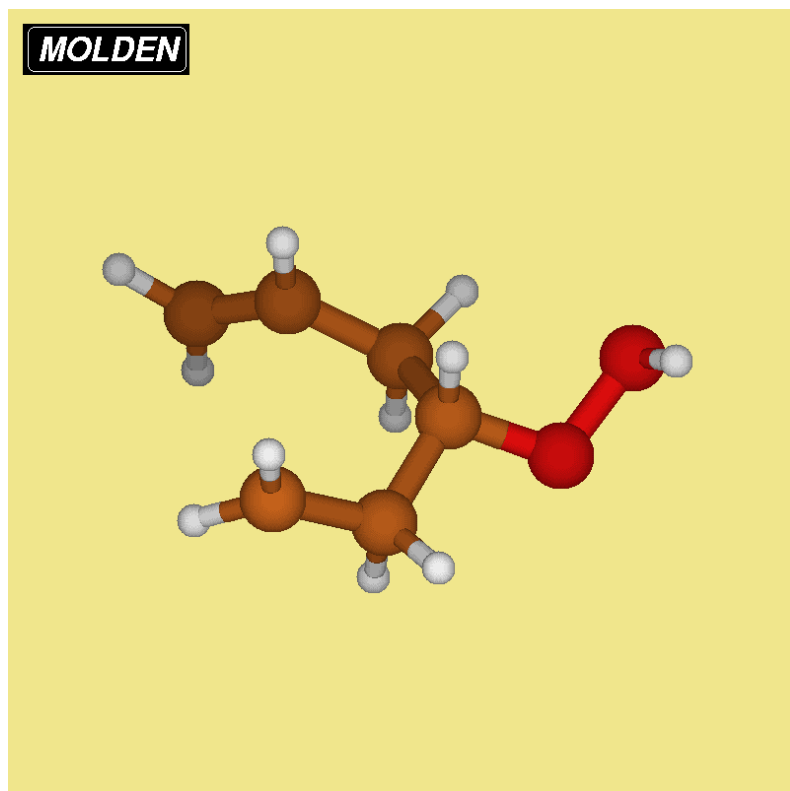
-417.8488	105.3185	125.6443
181.1556	207.7305	242.2161
295.6237	352.0518	400.9752
443.7730	465.0365	506.8150
539.2275	674.8196	736.8322
831.9042	866.7239	922.6831
930.2497	931.7066	963.9381
973.1459	1021.8205	1029.9613
1069.9910	1105.3483	1174.8128
1212.9800	1265.5972	1284.8014
1300.3447	1322.2261	1360.1975
1388.6494	1396.6540	1444.3726
1475.2027	1490.6822	1508.0700
1604.7414	2972.5910	3003.5855
3045.5927	3055.4099	3116.3322
3135.3093	3148.6876	3162.0517
3229.5057	3234.3939	3751.9319

Rotational constants (GHZ): 3.50200 1.36866 1.06273

\*\*\*\*\*

inter 2: CH<sub>2</sub>CH<sub>2</sub>CH(OOH)CH<sub>2</sub>CHCH<sub>2</sub>





C	0	0.16065	0.30312	-0.19888
C	0	0.24776	-0.3358	1.19572
C	0	1.36156	0.1944	2.05356
C	0	2.2584	-0.55376	2.69876
C	0	2.61308	0.598	-0.79468
C	0	1.32653	-0.06747	-1.14566
H	0	0.3324	-1.423	1.08275
H	0	2.25952	-1.63822	2.61891
H	0	3.46247	0.03763	-0.42596
H	0	1.00729	0.22695	-2.157
H	0	-0.71252	-0.13711	1.68837
H	0	1.43751	-1.1571	-1.15335
H	0	2.70523	1.67794	-0.85528
H	0	3.02073	-0.11103	3.33265
H	0	1.39807	1.2781	2.17297
O	0	-1.00845	-0.15483	-0.89475
O	0	-2.17913	0.33801	-0.18247
H	0	-2.48332	1.01325	-0.81107
H	0	0.10434	1.39856	-0.10476

Frequencies:

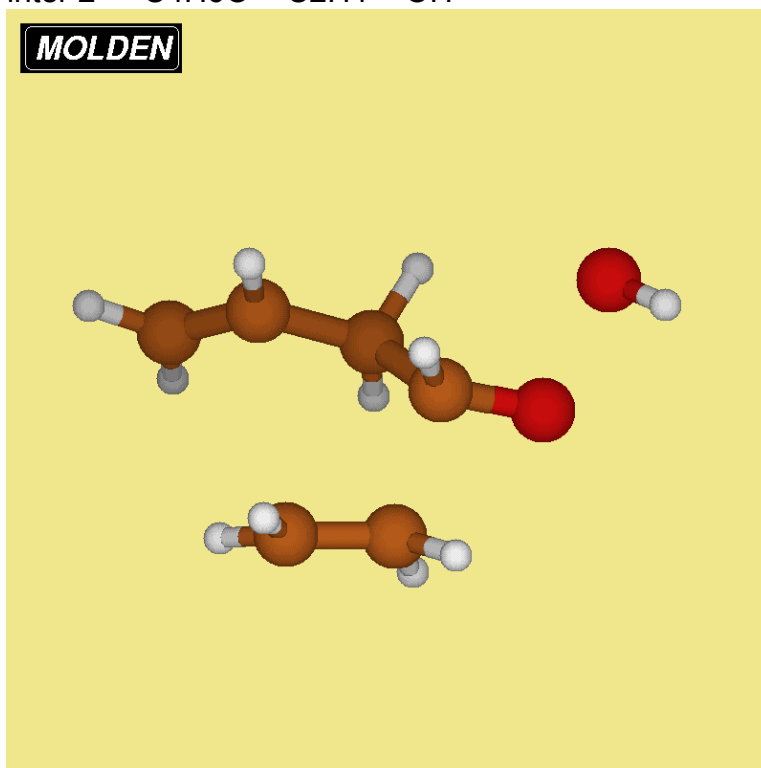
55.4286	91.5263	97.8925
119.3182	134.4098	186.8603
209.3216	241.1267	312.6097

375.8925	427.9999	459.0944
485.9994	542.7672	624.2568
794.9939	866.9984	924.3965
930.8844	936.1891	963.2998
1024.0361	1029.6458	1065.5796
1081.9635	1104.7633	1181.4350
1230.7030	1273.5503	1302.2107
1314.4426	1333.8563	1359.4418
1372.6847	1406.7078	1465.4935
1479.8103	1489.1828	1500.0048
1721.9977	3001.4144	3004.4985
3041.1965	3085.4530	3090.0639
3136.2520	3151.3346	3166.0751
3235.2591	3277.7087	3750.2409

Rotational constants (GHZ):      2.66799    1.35474    0.97506

\*\*\*\*\*

inter 2 -> C4H6O + C2H4 + OH



C	0.0517807821	0.3594228432	-0.1357609268
C	0.2857020643	-0.3601432987	1.1897392845
C	1.3527629076	0.226935199	2.0637198546
C	2.2948859727	-0.4676563816	2.7052349556
C	2.6843112973	0.4161438612	-0.7887241863
C	1.4853124178	-0.0451425302	-1.3442408767

H 0.4470215567 -1.4294052425 1.0153041011  
H 2.3684986291 -1.5488485886 2.6130085965  
H 3.2756234539 -0.1984454383 -0.1210558397  
H 1.0908028481 0.4969597081 -2.1994763504  
H -0.6871878315 -0.2696566268 1.6973012678  
H 1.341988087 -1.1210662888 -1.4080975428  
H 2.9891428965 1.4529215225 -0.8968818951  
H 3.0173284162 0.0159178694 3.3557956877  
H 1.3120691845 1.30853848 2.2016415916  
O -0.9412700692 -0.0728258433 -0.8664120102  
O -2.4379246652 0.4473658725 -0.0336980217  
H -2.7833476949 0.8237649606 -0.8601633397  
H 0.1646257469 1.4528569223 -0.0673963501

Frequencies:

-832.5274	52.3193	76.9144
89.9745	103.7250	146.6838
153.3366	197.7470	251.4163
302.9095	359.7067	393.5133
418.5968	480.1942	509.8533
619.8158	811.8036	821.9935
881.2225	917.5463	940.0488
943.5497	961.8356	1030.3766
1049.1735	1053.9726	1129.5360
1166.3413	1210.8386	1248.4096
1256.8588	1290.8162	1316.9411
1336.7202	1438.7610	1459.3297
1477.8828	1483.8825	1554.4625
1721.6064	2998.1733	3018.6227
3088.7999	3135.3546	3136.0786
3150.0165	3168.4328	3217.8245
3235.0723	3273.2779	3784.8470

Rotational constants (GHZ): 2.45220 1.30007 0.91208

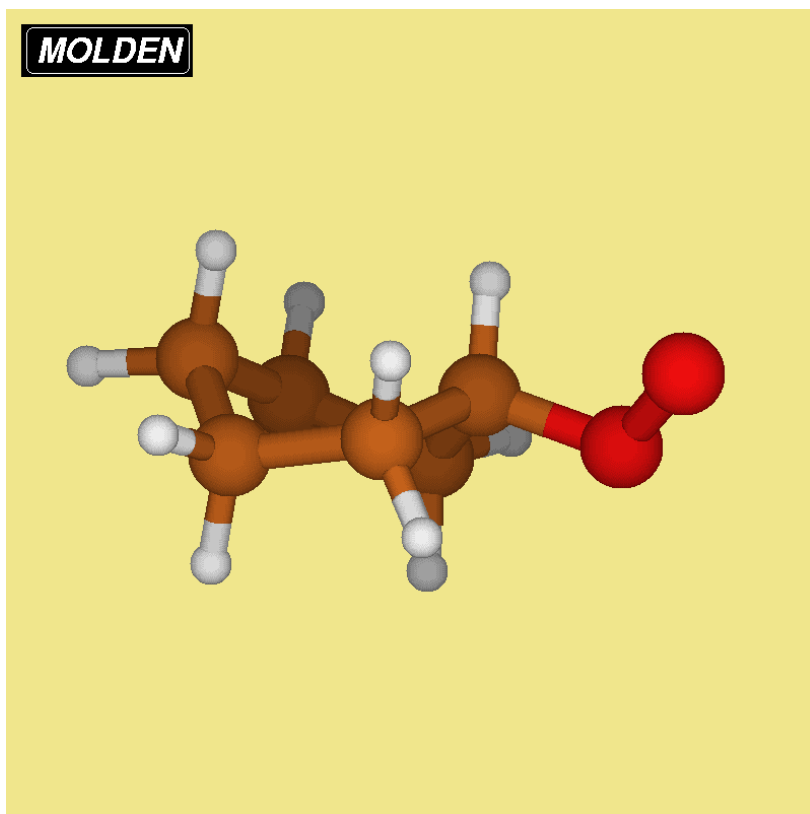
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boat - chair transformations

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cyC6OO\_eq\_boat



```
C -0.6189641532 -0.9975024967 0.4177169937
C 0.2954654103 -0.2370907288 -0.5590852337
C 0.0489767307 1.2652802568 -0.5200357497
C 0.4361195809 1.8297513299 0.8703287846
C 0.2225675146 0.8028087307 2.0095967898
C -0.9274733281 -0.1600407769 1.682624026
O 0.037398795 -0.6808775005 -1.9332559671
O 0.522139147 -1.8939842454 -2.1490824431
H -1.0123068241 1.4485394988 -0.7258672158
H 1.1407137323 0.2209218203 2.1633790244
H -1.1272556971 -0.826139887 2.5282996473
H -0.1461841139 -1.9484851983 0.6801194356
H 0.6149441814 1.7618570045 -1.3140285266
H -1.5477066434 -1.2412473754 -0.109464447
H -1.844637896 0.42209391 1.5281732212
H 0.0319982989 1.3246064059 2.9533563937
H -0.1597723708 2.7289600258 1.0602899288
H 1.48341077 2.1513806967 0.8606683108
H 1.3503424967 -0.4628308227 -0.3730921556
```

Frequencies:

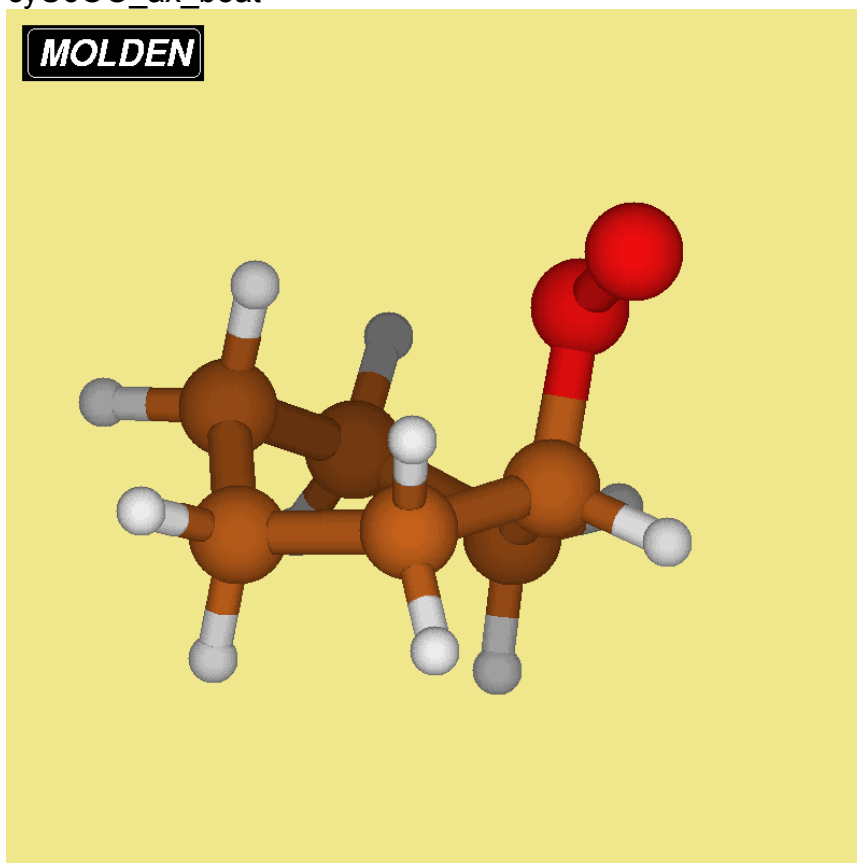
63.2762	78.6468	152.4901
237.2694	266.2536	365.5382
428.2232	467.0167	511.3600

582.9069	772.4447	793.1606
848.1418	896.9287	909.1240
931.1788	941.4171	1026.3675
1048.6662	1086.9452	1108.3999
1120.0392	1173.7536	1198.9213
1209.5616	1257.3281	1290.8364
1300.2618	1322.8801	1338.4543
1369.6799	1372.8782	1385.2126
1388.8535	1400.2697	1500.3293
1503.0534	1512.0179	1516.8487
1532.0703	3031.5257	3041.3656
3048.9429	3054.2992	3063.3471
3076.8815	3079.9365	3087.4687
3094.0674	3107.3130	3115.1442

Rotational constants (GHZ):        3.91935    1.39043    1.13893

\*\*\*\*\*

cyC6OO\_ax\_boat



C -0.9915945551 -1.0376813091 0.0400912638  
C -0.1102709589 -0.3018095435 -0.9816057793  
C -0.2811452842 1.2119157674 -0.9286833677  
C 0.0442500022 1.7995543319 0.4683005018

C -0.1956461747 0.7892249618 1.6139974576  
C -1.3393221072 -0.175068709 1.2723637263  
O 1.3259515115 -0.5381481521 -0.7013172092  
O 1.6581790217 -1.8053066686 -0.8657240566  
H -1.3265048227 1.4147061421 -1.1910746764  
H 0.7170070049 0.207520558 1.7880302411  
H -1.5678670556 -0.8246102407 2.1239920224  
H -0.4599071794 -1.950346078 0.3274056243  
H 0.3308442383 1.6865397339 -1.7021406945  
H -1.9082941279 -1.3630160616 -0.4645296323  
H -2.2510153367 0.4048098487 1.0762634981  
H -0.4077792214 1.3244178613 2.5458177751  
H -0.5742847665 2.6911301517 0.6219095673  
H 1.08470583 2.137075059 0.4928160672  
H -0.2675743607 -0.6974014059 -1.9889424809

Frequencies:

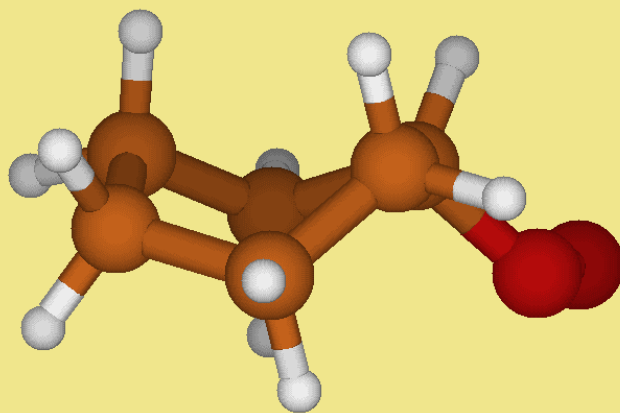
78.2662	104.3510	144.2930
248.5237	297.7034	340.6635
445.1584	475.3686	537.2743
673.6364	768.2194	793.8095
808.8509	866.5097	878.9394
910.9039	937.1831	1011.7872
1046.3402	1056.6294	1114.5829
1136.4819	1161.1565	1186.1237
1211.4127	1272.8889	1276.0707
1303.5940	1341.0438	1352.0884
1356.6663	1369.5293	1390.8290
1395.1984	1397.9777	1491.6511
1495.5734	1506.3902	1511.7217
1525.2929	3031.3304	3046.8654
3049.1279	3057.2299	3057.8274
3082.3226	3084.9623	3091.3833
3096.0382	3106.2004	3109.4102

Rotational constants (GHZ): 3.03381 1.70613 1.47646

\*\*\*\*\*

cyC6OO\_eq\_boat\_O2lat

**MOLDEN**



```
C 0.0146858358 -0.3533178523 -0.8027759499
C 0.0132081122 1.1827753073 -0.7741882784
C 0.1672935672 1.7293551511 0.6504167158
C -1.0029688771 1.2763516999 1.5552444242
C -1.534089201 -0.1272132013 1.1689640414
C -0.4361247306 -0.9837320352 0.5228546193
H -0.9300604024 1.5365271813 -1.2074273191
H -1.8225413446 2.0018063726 1.4964847512
H -2.371204664 -0.0312892022 0.4652707333
H 0.4318646219 -1.0389628784 1.1908832151
H 0.8115254398 1.5455283708 -1.4305101869
H -0.7673014833 -2.010961874 0.3512351608
H -1.9388067087 -0.6372685067 2.0490048337
H -0.6694747852 1.2746516117 2.5991388785
H 0.2338055611 2.8221328467 0.6328656196
H 1.1189846423 1.3728066877 1.0620277457
H -0.5770757301 -0.7333434643 -1.6410778902
O 1.4033304278 -0.7551248412 -1.0934719946
O 1.490201649 -2.050742854 -1.3429016274
```

Frequencies:

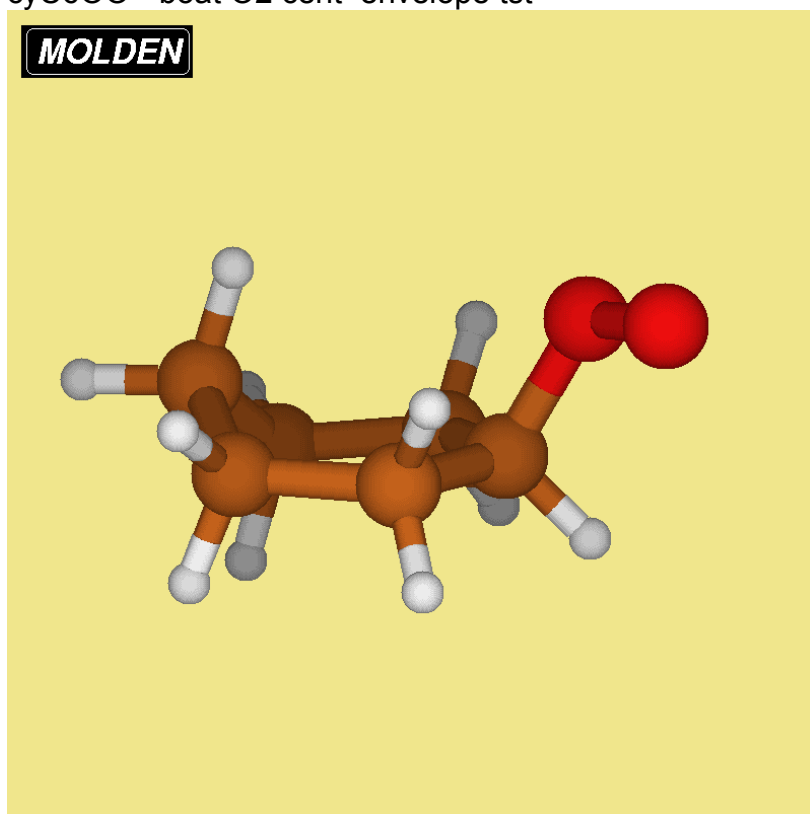
55.2702	88.0821	179.1527
238.1416	296.0206	367.0223

405.4979	500.6039	534.5547
591.4893	774.4692	787.4213
825.1980	876.8806	895.9697
908.6838	969.1745	1018.2641
1033.4027	1082.3639	1115.1128
1138.2928	1150.5036	1195.8814
1206.4751	1247.6072	1278.3409
1303.5058	1331.3494	1344.4904
1362.9552	1381.4425	1382.6946
1392.4983	1393.0056	1489.7922
1501.4631	1507.4729	1517.0729
1528.1642	3033.4098	3042.3432
3048.5447	3050.7660	3056.8181
3076.1139	3082.5021	3090.5476
3094.9578	3101.2858	3117.8999

Rotational constants (GHZ):        3.87286    1.44004    1.18371

\*\*\*\*\*

cyC6OO->boat O2 cent envelope tst



C 0.7361868376 -0.279308425 0.5027986813  
C -0.2761106878 -1.4340799577 0.3348279444  
C -1.7546873435 -1.0258050463 0.231840517  
C -1.9197539068 0.264161552 -0.5748572843



C -1.2699743564 1.4175433692 0.1946750191  
C 0.2277675181 1.1840522902 0.5035077242  
H -0.1368411614 -2.1599661444 1.1421418574  
H -2.9807472066 0.4796979487 -0.7442555344  
H -1.8220890332 1.5436235833 1.1349116314  
H 0.8516292439 1.7159245299 -0.2202043076  
H 0.0086133406 -1.9521540456 -0.588541956  
H 0.4698340122 1.6302258097 1.47301254  
H -1.3801617398 2.361025203 -0.3507583426  
H -1.4565100148 0.1502880128 -1.5648480389  
H -2.1774945521 -0.8692763565 1.2334201111  
H -2.3192413168 -1.851263927 -0.2155380511  
H 1.3753193539 -0.4421115964 1.3733469282  
O 1.6624811384 -0.4718859337 -0.6528156092  
O 2.7259089501 0.3012114697 -0.5758646968

Frequencies:

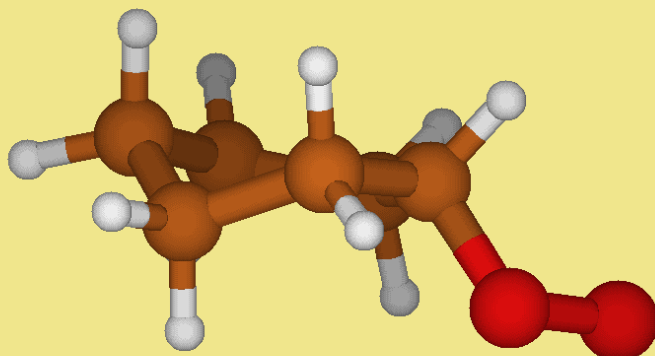
-131.8632	49.1830	101.9106
283.4340	304.2341	369.8635
439.1402	470.1115	516.1411
637.3287	762.1901	770.2567
802.0352	873.5287	895.8515
911.6841	938.6304	1003.1947
1063.1302	1074.9541	1132.5418
1145.2736	1161.5208	1199.2450
1211.7963	1277.2548	1302.2385
1309.9289	1332.9981	1338.3824
1359.5009	1389.8452	1393.0902
1393.8630	1409.2022	1495.3875
1498.4506	1506.4489	1509.9292
1525.8992	3025.9430	3030.2835
3035.2891	3050.2589	3067.2269
3077.8317	3079.6712	3082.1376
3091.1212	3103.5074	3113.8693

Rotational constants (GHZ): 3.48317 1.50116 1.21669

\*\*\*\*\*

cyC6OO ->boat O2 lat envelope tst

**MOLDEN**



```
C 0.6933091973 -0.1743748347 0.5381224817
C -0.2863045766 -1.3508985591 0.4342506789
C -1.4798642499 -1.0783517921 -0.4838929661
C -2.2286784022 0.1517014533 0.0347335966
C -1.3640964105 1.4241098475 -0.0582331533
C 0.1715598204 1.2273582783 0.1304431856
H -0.6637295346 -1.5733797234 1.439990001
H -2.5133553825 -0.036664873 1.0791230977
H -1.7315371628 2.1612631737 0.6630129738
H 0.6736773471 1.4651487104 -0.8108233781
H 0.2812647992 -2.2315985371 0.1141646763
H 0.5513554129 1.9572624032 0.8491830546
H -1.5196249613 1.87272031 -1.0455488225
H -3.1636690902 0.3071140211 -0.5145593948
H -2.1374018375 -1.9545031516 -0.5026977537
H -1.1408891202 -0.9144082247 -1.5155739835
H 1.1488098981 -0.142383793 1.5312847245
O 1.8135341128 -0.5466224382 -0.3613343264
O 2.8339093074 0.2831428539 -0.2461779406
```

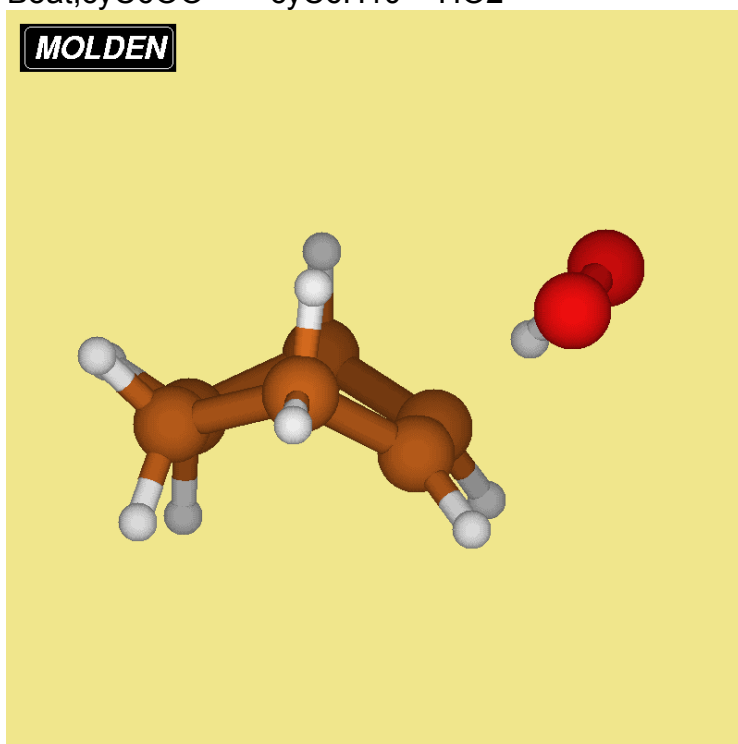
Frequencies:

-187.8656	27.5114	84.4453
251.0767	304.7667	368.9936
430.0233	484.6172	528.5527

646.7137	749.5568	765.5749
810.1586	873.5740	894.6735
920.0993	939.7895	1003.9776
1053.4923	1089.4932	1131.5752
1142.5386	1162.4926	1201.3927
1212.9903	1283.4935	1299.8152
1307.0128	1322.8091	1351.9732
1362.7987	1381.5178	1391.9232
1396.1631	1406.1730	1490.6617
1496.6202	1508.2120	1512.6573
1528.1859	3023.9009	3035.9318
3043.5358	3048.0673	3075.3900
3081.3558	3084.2602	3086.2174
3091.0689	3094.1554	3124.1606

Rotational constants (GHZ):            3.75664    1.44716    1.15507

Boat;cyC6OO <-> cyC6H10 + HO2



C	-0.467596	1.363563	-0.158958
C	-0.825835	-1.378746	-0.295055
C	0.222703	-0.862580	0.691446
C	-1.963620	0.930183	-0.181092
C	-2.152523	-0.609740	-0.109846
C	0.312387	0.523546	0.808304

H	0.396630	-1.453521	1.592876
H	-2.485352	1.404371	0.656618
H	-2.882125	-0.938358	-0.858137
H	0.759755	0.984144	1.682662
H	-0.374837	2.429896	0.063096
H	-0.984484	-2.452784	-0.158821
H	-0.472880	-1.250305	-1.327056
H	-0.051039	1.216679	-1.162802
H	1.430215	-0.995180	0.091082
H	-2.418045	1.332509	-1.092805
H	-2.566134	-0.882871	0.867588
O	2.506285	-0.574571	-0.426373
O	2.355616	0.675578	-0.184015

---

Rotational constants (GHZ):	3.6104559	1.3853980	1.1392515
Frequencies --	-1052.0676	83.8196	116.8609
Frequencies --	148.9693	194.7057	258.8356
Frequencies --	361.8920	460.6110	485.5358
Frequencies --	564.4291	618.0004	681.1347
Frequencies --	771.0640	819.4607	826.0221
Frequencies --	891.9340	932.0062	955.3008
Frequencies --	971.6127	984.1312	1040.0370
Frequencies --	1069.7757	1126.3505	1138.0282
Frequencies --	1204.1219	1231.1883	1264.4109
Frequencies --	1272.2371	1287.9931	1328.5860
Frequencies --	1337.4897	1344.5208	1369.6780
Frequencies --	1383.4700	1409.5020	1493.0021
Frequencies --	1504.8917	1510.0982	1525.2129
Frequencies --	1549.4583	1597.7042	3032.3737
Frequencies --	3043.7790	3046.6986	3058.1104
Frequencies --	3079.3972	3094.7023	3100.5792
Frequencies --	3112.4484	3123.8001	3210.2770