

Ab Initio Kinetics Studies of Hydrogen Atom

Abstraction from Methyl Propanoate

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Table S1. Optimized geometries, rotational constants, and vibrational frequencies with internal rotations projected out of the reactants, transition states (TSs), and products obtained using DFT-M08-HX/cc-pVTZ. The parameters V_i ($i = 0 - 10$) for rotational potential energy surfaces fitted with $V = V_0 + V_1 \cos(\Delta\theta) + V_2 \cos(2\Delta\theta) + V_3 \cos(3\Delta\theta) + V_4 \cos(4\Delta\theta) + V_5 \cos(5\Delta\theta) + V_6 \sin(\Delta\theta) + V_7 \sin(2\Delta\theta) + V_8 \sin(3\Delta\theta) + V_9 \sin(4\Delta\theta) + V_{10} \sin(5\Delta\theta)$ are also given in order.

CH₃CH₂C(=O)OCH₃:

Cartesian Coordinates (Å)

C	-1.0677423119	2.4105439860	-1.8542930641
C	-1.2647107522	0.9944325436	-1.3403133179
C	-0.0562058055	0.4931450439	-0.5918147255
O	0.9541231819	1.1139319606	-0.4078035980
O	-0.2376698043	-0.7556522633	-0.1417378804
C	0.8663150875	-1.2975348309	0.5780219624
H	-0.2085711199	2.4611463547	-2.5261812951
H	-1.9529033227	2.7548356398	-2.3925093894
H	-0.8723526554	3.0972413346	-1.0281616096
H	-2.1237517625	0.9192081125	-0.6652807518
H	-1.4646486871	0.2875693330	-2.1524803684
H	1.0862762352	-0.6869932460	1.4569974231
H	1.7566338431	-1.3290378090	-0.0544813219
H	0.5727317838	-2.3030750093	0.8748399166

Frequencies (cm⁻¹):

211.16 342.88 451.85 594.82 666.57 806.52 878.46 1003.95 1045.99 1113.16
 1117.73 1207.20 1219.70 1248.27 1274.23 1388.79 1407.19 1450.01 1465.57 1474.28
 1477.36 1485.50 1488.54 1842.54 3048.88 3049.96 3052.40 3090.25 3129.56 3133.29
 3135.11 3166.43

Rotational constants (GHz): 9.66885 2.17135 1.83337

V_i ($i = 0 - 10$) (cm⁻¹) for rotations:

HC3-C2C1: 352.55 2.53 -3.79 -358.81 3.84 -2.26 -0.11 0.02 0.00 -0.02 0.11
 C3C2-C1O1: 362.16 -152.57 -134.27 -72.08 -2.99 1.94 0.00 -0.01 0.00 0.02 0.01
 C2C1-O2C4: 2864.50 -1123.42 -1663.46 -117.48 37.14 -29.65 0.00 0.00 -0.02 -0.01 -0.01
 C1O2-C4H: 200.90 -0.88 -1.26 -188.14 1.02 0.72 -1.40 2.01 0.00 1.94 -1.41

CH₃CH₂C(=O)OCH₂:

Cartesian Coordinates (Å)

C	-1.0659467212	2.4023774746	-1.8540730004
C	-1.2416806875	0.9897339718	-1.3229276117
C	-0.0187928988	0.5103207732	-0.5903606060
O	0.9919202592	1.1274627954	-0.4245112684
O	-0.1986028557	-0.7513359210	-0.1206604122

C	0.8266897147	-1.3247365486	0.5626634735
H	-0.2182093426	2.4541475658	-2.5402483594
H	-1.9627438597	2.7314428928	-2.3820862641
H	-0.8656375311	3.0997858536	-1.0382048661
H	-2.0896293303	0.9126703936	-0.6338639658
H	-1.4471634651	0.2722452724	-2.1246201538
H	0.6181921728	-2.3140405650	0.9296461230
H	1.7244376956	-0.7518624085	0.7241927312

Frequencies (cm⁻¹):

56.35 102.71 152.91 213.73 216.52 280.04 362.97 462.93 577.49 663.70 807.41
 859.54 1013.64 1089.29 1108.38 1158.52 1197.58 1272.93 1275.79 1388.09 1412.74
 1452.09 1454.85 1483.21 1491.92 1862.47 3061.66 3064.67 3098.93 3146.30 3149.86
 3219.55 3377.42

Rotational constants (GHz): 9.88174 2.24964 1.87456

CH₃CHC(=O)OCH₃:

Cartesian Coordinates (Å)

C	-1.0755276004	2.4299527174	-1.8974516884
C	-1.0591535405	1.0175565811	-1.4672645720
C	-0.0408049660	0.5346256906	-0.5590745153
O	0.8480326910	1.2102952821	-0.0904264892
O	-0.1848558513	-0.7754812265	-0.2808126886
C	0.7927789837	-1.2994965608	0.6089992131
H	-0.9934053425	2.5118294397	-2.9881326734
H	-2.0201449946	2.9155211761	-1.6235972790
H	-0.2500656463	2.9751615002	-1.4371737590
H	-1.8009628576	0.3101488595	-1.8156028096
H	0.7588184264	-0.7766176289	1.5682278027
H	1.7953692438	-1.1850204298	0.1889990262
H	0.5522971844	-2.3534360806	0.7404433623

Frequencies (cm⁻¹):

94.43 113.62 160.32 200.36 217.02 349.56 471.10 575.95 679.30 749.35 880.61
 988.70 1031.03 1082.36 1166.73 1182.21 1213.57 1243.56 1388.06
 1428.87 1464.19 1465.05 1473.73 1492.11 1508.35 1761.41 3023.83 3057.54
 3074.85 3134.99 3149.43 3176.08 3229.44

Rotational constants (GHz): 10.24225 2.18459 1.84174

CH₂CH₂C(=O)OCH₃:

Cartesian Coordinates (Å)

C	-1.0044322529	2.3962629334	-1.8979165999
C	-1.2385116188	1.0664658049	-1.2920270779
C	-0.0067494120	0.4962545797	-0.6291842800
O	1.0672409565	1.0259241070	-0.5732255749
O	-0.2595428865	-0.7047952966	-0.0949789708
C	0.8530411340	-1.3161832220	0.5532088187
H	-0.0259044453	2.8484541994	-1.8330608279

H	-1.8075106944	2.9117939572	-2.4031703036
H	-2.0364623296	1.0850186265	-0.5348039089
H	-1.5850219268	0.3252492223	-2.0276095713
H	1.2107370021	-0.6871339099	1.3716836987
H	1.6719745884	-1.4656912736	-0.1542924025
H	0.4964156353	-2.2720778484	0.9330940404

Frequencies (cm⁻¹):

57.42 152.97 168.57 172.62 224.53 355.39 449.05 462.34 583.37 661.09 875.99
 915.64 1017.47 1047.72 1137.24 1181.87 1189.30 1212.06 1253.77
 1397.51 1430.81 1449.33 1473.87 1475.34 1493.44 1855.22 3010.27 3031.17
 3062.44 3142.44 3180.60 3196.26 3311.79

Rotational constants (GHz): 9.92294 2.26296 1.88542

H + CH₃CH₂C(=O)OCH₃ → Products

H₂:

Cartesian Coordinates (Å)

H	0.0000000000	0.0000000000	-0.3718384726
H	0.0000000000	0.0000000000	0.3718384726

Frequencies (cm⁻¹): 4431.19

Rotational constants (GHz): 0.00000 1811.73862 1811.73862

TS- α [H]:

Cartesian Coordinates (Å)

C	-2.16778779	0.96894550	-0.19101888
C	-1.10598457	-0.05042262	-0.50871968
C	0.25437772	0.28808063	-0.00346580
O	0.49611333	1.15294683	0.79588866
O	1.19142163	-0.51763558	-0.51999545
C	2.51129293	-0.28161883	-0.03739132
H	-2.00420403	1.88725793	-0.76317096
H	-3.16159868	0.58758426	-0.43346432
H	-2.13414931	1.23453677	0.86722684
H	-1.39523745	-1.09891474	0.11465342
H	-1.07919574	-0.40882388	-1.53789926
H	2.55021811	-0.41236949	1.04665816
H	2.82885957	0.73609000	-0.27658403
H	3.15162277	-1.00878513	-0.53388900
H	-1.70815790	-1.93389153	0.63251334

Frequencies (cm⁻¹): 1872.36i

209.97 280.12 329.74 343.91 459.39 660.30 690.26 840.70 880.78 1017.37 1046.66
 1079.54 1123.32 1204.07 1213.14 1217.50 1245.22 1294.75 1351.823 1387.05
 1407.59 1464.75 1469.77 1473.75 1479.78 1487.66 1823.95 3041.14 3049.11 3114.02
 3126.58 3129.87 3142.39 3167.16

Rotational constants (GHz): 8.42964 2.10428 1.80533

V_i ($i = 0 - 10$) (cm⁻¹) for rotations:

HC3-C2C1: 257.93 2.51 -3.13 -264.89 3.03 -2.48 3.21 -1.40 -7.33 -1.25 3.33
 C3C2-C1O1: 753.40 -149.13 -543.23 -57.74 -5.29 -0.92 86.36 -189.88 35.82 14.13 0.35
 C2C1-O2C4: 2827.84 -1090.50 -1621.22 -130.63 20.43 -22.64 -103.53 -65.86
 -41.45 -13.80 36.49
 C1O2-C4H: 200.08 1.68 2.42 -187.55 -2.13 -1.53 0.00 -0.06 3.06 0.01 0.07

TS- β [H]:

Cartesian Coordinates (Å)

C	-2.02411056	-0.74389565	-0.42034245
C	-0.68395084	-1.17605758	0.10016403
C	0.38938046	-0.15643123	-0.19562243
O	0.25473219	0.80428803	-0.90064937
O	1.53743231	-0.46181494	0.41884425
C	2.60765743	0.44700667	0.17036633
H	-2.01130700	-0.32962635	-1.42579877
H	-2.83794880	-1.44290602	-0.24246463
H	-2.35565042	0.30929008	0.31581029
H	-0.70000082	-1.35289943	1.18053365
H	-0.35969356	-2.12449336	-0.34888291
H	2.33778167	1.45235813	0.50147462
H	2.83844590	0.48185092	-0.89688945
H	3.46078038	0.07400515	0.73429334
H	-2.50737953	1.03577995	0.90372258

Frequencies (cm^{-1}): 1006.19i

211.99 280.79 352.22 456.94 527.89 597.09 673.18 855.94 881.57 1009.01 1043.82
 1079.61 1117.09 1191.62 1206.14 1209.17 1220.54 1234.37 1255.23 1394.68 1432.07
 1441.42 1467.71 1474.37 1487.12 1638.12 1845.01 3027.73 3050.90 3082.62 3111.78
 3132.16 3168.93 3204.10

Rotational constants (GHz): 8.65411 2.08978 1.80350

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 413.99 98.44 -224.27 -303.30 -8.31 12.31 -221.36 -235.04 112.83 61.10 14.56
 C3C2-C1O1: 447.40 -119.66 -263.07 -62.98 -3.56 -3.03 46.08 17.94 -33.49 -16.39 -5.14
 C2C1-O2C4: 2905.67 -1156.94 -1657.85 -123.73 32.48 -27.45 -22.04 23.96 22.04 2.22 -
 6.92
 C1O2-C4H: 200.28 1.67 2.37 -187.78 -2.16 -1.47 -0.03 0.04 1.43 0.04 0.02

TS-m [H]:

Cartesian Coordinates (Å)

C	-2.50819159	0.10746580	0.01125419
C	-1.26172149	-0.75562549	0.11042362
C	-0.00417489	0.05276872	-0.06113186
O	0.05306158	1.23266721	-0.25358182
O	1.09638333	-0.72726679	0.02525387
C	2.31632304	-0.06790686	-0.10871117
H	-2.55745935	0.60489875	-0.95947564
H	-3.40828252	-0.49640331	0.13993187

H	-2.49889040	0.88765347	0.77500963
H	-1.19196498	-1.26711273	1.07631862
H	-1.24922454	-1.54836476	-0.64519507
H	2.51209903	0.60902423	0.97306120
H	2.32034588	0.68191892	-0.89929664
H	3.11455536	-0.80368674	-0.15720512
H	2.56312299	1.08979213	1.83574259

Frequencies (cm⁻¹): 1616.25i

213.28 341.74 360.42 457.46 512.32 604.39 669.34 805.01 870.54 1008.84 1072.19
 1112.30 1132.57 1152.30 1193.06 1224.12 1273.00 1275.08 1297.06 1386.76 1407.95
 1447.56 1449.23 1458.75 1477.81 1486.11 1853.00 3050.16 3052.52 3089.99 3096.24
 3133.90 3136.67 3208.62

Rotational constants (GHz): 8.76128 2.07632 1.78720

V_i ($i = 0 - 10$) (cm⁻¹) for rotations:

HC3-C2C1: 357.39 -1.27 1.68 -362.72 -1.80 1.11 2.02 3.12 -2.01 3.23 1.80

C3C2-C1O1: 379.19 -155.59 -129.63 -86.06 -5.34 2.08 5.52 -1.32 -1.99 -0.18 0.45

C2C1-O2C4: 2566.66 -948.87 -1558.53 -103.76 40.83 -17.40 -218.01 -23.70 39.14 4.63
 34.18

C1O2-C4H: 552.06 -29.36 -459.32 -169.77 52.21 40.35 -40.99 -301.27 168.85 65.30 -9.39

CH₃ + CH₃CH₂C(=O)OCH₃ → Products

CH₃:

Cartesian Coordinates (Å)

C	0.0000715227	-0.0000002118	0.0001265099
H	0.5395818855	-0.9347541331	0.0001297230
H	0.5395815389	0.9347540819	0.0001297415
H	-1.0792349071	0.0000002634	-0.0001257344

Frequencies (cm⁻¹):

521.25 1406.11 1406.52 3139.61 3320.32 3320.95

Rotational constants (GHz): 286.76762 286.68794 143.36389

CH₄:

Cartesian Coordinates (Å)

C	-0.0000001248	-0.0000007897	-0.0000015848
H	0.6294383827	-0.6294376083	-0.6294369676
H	-0.6294376485	0.6294381016	-0.6294363943
H	-0.6294369710	-0.6294363575	0.6294378585
H	0.6294363616	0.6294366538	0.6294370882

Frequencies (cm⁻¹):

1325.18 1325.18 1325.19 1549.76 1549.77 3043.55 3169.62 3169.62 3169.62

Rotational constants (GHz): 158.06654 158.06632 158.06615

TS- α [CH₃]:

Cartesian Coordinates (Å)

C	2.1121818894	1.0772604603	0.2619444342
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C	1.0539658007	0.0681153580	0.6214570396
C	-0.2739856620	0.3106659802	0.0104989818
O	-0.4975407087	1.0791961732	-0.8890284726
O	-1.2207773213	-0.4813767889	0.5431556307
C	-2.5120362794	-0.3359835584	-0.0383899081
H	1.9084698116	2.0460150173	0.7292874249
H	3.0993591267	0.7435577312	0.5893728552
H	2.1309762808	1.2374670279	-0.8181842282
H	1.4015835411	-1.0528314314	0.1026022519
H	0.9778031702	-0.1941367851	1.6764609379
H	-2.4812662447	-0.5705906159	-1.1052753931
H	-2.8721988319	0.6888966611	0.0798666913
H	-3.1639253134	-1.0322107652	0.4871776129
C	1.7986359759	-2.2797897159	-0.4896757869
H	2.5957539828	-2.6297418542	0.1585716093
H	2.1089279173	-1.9799602919	-1.4857457974
H	0.8789895749	-2.8548843324	-0.4433688534

Frequencies (cm^{-1}): 1765.01i

104.70 172.78 210.34 338.28 440.05 457.31 502.51 548.75 684.63 740.55 872.99
 885.75 1025.35 1067.81 1088.57 1125.75 1137.86 1207.66 1211.49 1239.73 1308.54
 1362.51 1389.53 1407.91 1418.81 1422.02 1464.45 1467.27 1472.98 1481.18 1488.65
 1813.24 3035.28 3047.10 3078.13 3106.12 3124.30 3126.97 3137.59 3163.40 3231.54
 3232.79

Rotational constants (GHz): 3.13085 1.66761 1.27445

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 225.62 -3.61 -0.14 -233.83 0.15 3.40 0.62 2.78 -17.87 2.48 1.15 C3C2-C1O1:
 804.98 -111.99 -631.91 -58.75 4.88 -1.75 -22.45 -236.32 34.11 47.79 -3.51

C2C1-O2C4: 2770.11 -1072.73 -1562.52 -129.43 6.24 -21.78 -58.54 -123.62 -48.11 -18.51
 47.54

C1O2-C4H: 202.22 1.48 0.83 -189.08 -2.40 -2.59 -0.13 0.28 1.53 -1.61 1.91

TS- β [CH_3]:

Cartesian Coordinates ($\text{\AA}$)

C	1.8715285012	1.0591070436	-0.2487712856
C	0.5214334281	1.1922301852	0.3997892993
C	-0.4665397106	0.1824167050	-0.1308223242
O	-0.2524551785	-0.6080146440	-1.0083422955
O	-1.6449652468	0.2727035018	0.4982328801
C	-2.6359873933	-0.6462655209	0.0461928377
H	1.8422307812	1.0148475486	-1.3359450254
H	2.6218543369	1.7515629423	0.1280405060
H	2.3135138722	-0.1443332506	0.0919482657
H	0.5764499194	1.0623586087	1.4866395142
H	0.0783547719	2.1857059373	0.2483020782
H	-2.2953773984	-1.6748103635	0.1867994527
H	-2.8450680859	-0.4913167963	-1.0148983097

H	-3.5255479869	-0.4532098082	0.6434545088
C	2.6362920790	-1.4116021363	0.4678085812
H	1.9708140589	-2.0201291164	-0.1380804487
H	3.6893227526	-1.5122928761	0.2185785431
H	2.4325516992	-1.4544301105	1.5352517022

Frequencies (cm^{-1}): 1631.96i

121.46 210.16 335.10 348.46 440.74 504.33 537.02 601.52 650.28 713.12 869.04
 886.41 1010.77 1047.59 1096.63 1132.11 1161.69 1206.47 1219.24 1235.10 1254.42
 1358.88 1372.47 1396.55 1429.06 1433.90 1440.86 1443.46 1467.10 1474.45 1487.37
 1838.61 3024.39 3049.50 3067.66 3070.08 3100.90 3130.16 3167.01 3188.01 3206.46
 3218.54

Rotational constants (GHz): 4.12223 1.40996 1.21979

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 528.87 14.41 -177.99 -352.87 -12.16 6.23 51.12 215.34 -82.11 -79.08 6.52
 C3C2-C1O1: 414.74 -159.93 -156.16 -75.28 -9.86 -13.23 -18.97 90.58 8.11 -22.65 -11.08
 C2C1-O2C4: 2870.73 -1119.92 -1666.79 -116.22 34.66 -31.73 1.19 14.25 5.97 0.14 -2.71
 C1O2-C4H: 201.95 1.67 2.48 -189.19 -2.19 -1.54 0.03 0.03 -1.06 -0.01 0.02

TS-m [CH_3]:

Cartesian Coordinates ($\text{\AA}$)

C	2.7004249518	-0.6405757914	0.1072081655
C	1.6443416459	0.3529270536	0.5612681049
C	0.3294878308	0.1375203806	-0.1413549088
O	0.1120059387	-0.6969336385	-0.9749447526
O	-0.6005139790	1.0144529199	0.2775952771
C	-1.8629489373	0.8974198530	-0.3190087391
H	2.8710959257	-0.5578799955	-0.9681104121
H	3.6452778416	-0.4658218027	0.6252805674
H	2.3779268361	-1.6648002988	0.3055814933
H	1.4558456080	0.2885724031	1.6381519991
H	1.9500246923	1.3883266379	0.3764841672
H	-2.3933346555	-0.2206431475	0.1250575562
H	-1.8112637573	0.7751296935	-1.4008108144
H	-2.4851640627	1.7205210740	0.0225189011
C	-2.7722149665	-1.4464602510	0.6300031410
H	-2.7180718456	-1.3255526528	1.7086796180
H	-2.0284030326	-2.1177422178	0.2103970438
H	-3.7785892045	-1.5939720296	0.2476332023

Frequencies (cm^{-1}): 1793.15i

186.68 212.91 329.16 341.87 443.46 512.77 563.26 609.01 657.66 697.86 805.30
 877.54 1008.44 1065.93 1111.19 1123.22 1128.13 1180.75 1217.80 1250.28 1274.07
 1372.21 1387.08 1396.53 1407.74 1427.68 1439.77 1449.45 1466.00 1477.55 1486.45
 1839.17 3049.56 3051.72 3070.41 3089.53 3090.95 3132.83 3135.12 3202.62 3215.15
 3221.41

Rotational constants (GHz): 4.25890 1.36164 1.20850

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 355.49 2.46 -3.62 -361.54 3.80 -2.17 -0.07 0.11 2.55 0.03 -0.05 C3C2-C1O1:
 363.24 -151.91 -133.17 -74.20 -2.04 2.58 -1.27 -0.51 5.05 1.11 -0.57
 C2C1-O2C4: 2665.78 -1008.70 -1595.53 -127.01 64.76 -10.05 -22.26 -59.71 18.25 -13.72
 51.09
 C1O2-C4H: 665.51 -2.64 -411.43 -226.88 9.16 -9.38 8.30 -344.46 130.20 47.95
 -1.06

O + CH₃CH₂C(=O)OCH₃ → Products

OH:

Cartesian Coordinates (Å)

O 0.0000000000 0.0000000000 -0.0573439865

H 0.0000000000 0.0000000000 0.9100904452

Frequencies (cm⁻¹):

3824.10

Rotational constants (GHz): 0.00000 569.02073 569.02073

TS-*α* [O]:

Cartesian Coordinates (Å)

C 1.9389611107 1.3328227208 0.2368516587

C 0.9761044239 0.2444209597 0.6114774001

C -0.3892178927 0.3623063191 0.0189427810

O -0.6884399047 1.1340686013 -0.8514687424

O -1.2401480053 -0.5136965673 0.5595276682

C -2.5512499816 -0.4955448166 -0.0014932919

H 1.6615372741 2.2680098296 0.7361962123

H 2.9570043133 1.0762477979 0.5343484589

H 1.9071615673 1.5179567510 -0.8383259925

H 1.4073268636 -0.8290658436 0.0775056955

H 0.9562268202 -0.0537073972 1.6600454201

H -2.5089271921 -0.7192148381 -1.0699428260

H -3.0090169301 0.4872239044 0.1328097504

H -3.1186515521 -1.2587818011 0.5278515108

O 1.8942188054 -1.8433431699 -0.4676284036

Frequencies (cm⁻¹): 1462.60i

81.54 162.12 209.72 336.56 453.73 539.66 632.14 684.68 820.00 882.71 994.37

1028.21 1064.93 1108.80 1157.47 1205.49 1216.19 1226.56 1253.93 1383.10 1404.62

1461.46 1464.75 1472.82 1475.17 1486.04 1825.27 3033.83 3051.32 3109.25 3129.02

3132.76 3146.99 3171.02

Rotational constants (GHz): 3.40160 1.67990 1.30498

V_i ($i = 0 - 10$) (cm⁻¹) for rotations:

HC3-C2C1: 262.06 -6.94 0.99 -270.99 -1.28 6.55 -0.06 3.78 -38.77 3.24 1.64 C3C2-

C1O1: 791.27 -291.19 -498.74 -7.81 11.29 -62.30 -25.16 133.96 -154.09 77.14 -39.82

C2C1-O2C4: 2943.82 -1317.26 -1619.66 66.84 -89.28 15.26 -25.51 -383.87 131.95 3.68

8.68

C1O2-C4H: 196.26 -0.54 -1.44 -184.22 0.90 0.78 1.20 -1.89 4.49 -1.60 0.84

TS-β [O]:

Cartesian Coordinates (Å)

C	-2.0222771871	-0.7995172218	-0.4363265516
C	-0.6838403851	-1.2200727865	0.0917755787
C	0.3708019904	-0.1772178183	-0.1944276502
O	0.2064951249	0.7919245060	-0.8817077046
O	1.5261716174	-0.4703921515	0.4059312223
C	2.5731070882	0.4723438858	0.1793937530
H	-2.0256101802	-0.4352652348	-1.4617836790
H	-2.8572193455	-1.4513111314	-0.1890344273
H	-2.2867880728	0.3073888599	0.2237281685
H	-0.7085435017	-1.3979463580	1.1707566657
H	-0.3499496998	-2.1630052334	-0.3631543546
H	2.2770475475	1.4604396202	0.5384960251
H	2.7995154118	0.5406831662	-0.8870948262
H	3.4364084447	0.1058231748	0.7318372266
O	-2.3091507730	1.2525791927	0.9661695734

Frequencies (cm⁻¹): 1729.24i

113.36	215.42	341.33	398.99	457.97	553.87	605.89	668.61	826.95	879.06	1004.31
1030.82	1047.62	1106.94	1162.05	1198.71	1207.83	1220.47	1246.16	1263.81	1395.12	
1425.81	1438.64	1468.73	1474.45	1486.60	1842.34	3024.65	3051.92	3093.93	3108.58	
3134.14	3170.37	3202.84								

Rotational constants (GHz): 4.32030 1.49299 1.31695

 V_i ($i = 0 - 10$) (cm⁻¹) for rotations:HC3-C2C1: 467.15 50.69 -176.47 -327.52 -36.11 20.44 104.09 264.78 -36.36
-92.60 -10.29

C3C2-C1O1: 459.86 -106.42 -328.59 -38.67 23.37 -11.74 121.81 -2.94 -55.33 1.07 -3.87

C2C1-O2C4: 2907.31 -1155.16 -1622.56 -167.16 23.93 -4.06 -157.18 48.60 44.84
-30.93 -0.45

C1O2-C4H: 198.78 -0.69 -1.13 -186.59 0.93 0.73 1.39 -2.14 4.24 -1.95 1.25

TS-m [O]:

Cartesian Coordinates (Å)

C	-2.5054879324	0.1126000524	0.0098298786
C	-1.2612792428	-0.7531105619	0.1137592366
C	-0.0047353001	0.0473850408	-0.0782510493
O	0.0668781517	1.2256049116	-0.2601304829
O	1.0984243029	-0.7469551216	-0.0177539473
C	2.3098329608	-0.0964684763	-0.1509639293
H	-2.5638033739	0.5906732770	-0.9701331626
H	-3.4056386673	-0.4860367661	0.1594554091
H	-2.4855384203	0.9068300292	0.7585703184
H	-1.1835547196	-1.2448330821	1.0895170832
H	-1.2555622762	-1.5607438324	-0.6259006138
H	2.5066935483	0.5821409072	0.9329343979

H	2.3184355473	0.6779072236	-0.9185535690
H	3.1155522671	-0.8248619060	-0.1912990993
O	2.5457649045	1.1696908844	2.0113178497

Frequencies (cm^{-1}): 1659.79i

167.29	210.74	344.21	388.38	457.45	567.74	594.84	667.51	804.79	862.68	1009.20
1071.52	1086.88	1113.15	1143.41	1169.35	1217.18	1258.74	1273.88	1279.94	1384.57	
1408.46	1446.34	1451.70	1478.16	1486.00	1864.17	3050.38	3053.35	3090.13	3091.79	
3134.49	3138.57	3209.13								

Rotational constants (GHz): 4.65319 1.35086 1.22890

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 360.32 -1.34 1.28 -365.27 -1.53 1.17 1.69 3.09 -9.76 3.12 1.55

C3C2-C1O1: 394.66 -158.58 -122.65 -102.92 -7.67 1.28 18.72 -1.49 -16.49 -1.85 0.24

C2C1-O2C4: 2255.91 -845.29 -1397.06 -51.95 52.88 -16.36 -489.34 -71.21 93.77 40.76 18.18

C1O2-C4H: 711.41 -34.59 -546.18 -169.03 16.89 20.30 64.75 -461.27 84.45 98.69 -10.78

OH + CH₃CH₂C(=O)OCH₃ → Products

H₂O:

Cartesian Coordinates (Å)

O	-0.3550704100	0.3846102556	0.0295304376
H	-0.3550704100	1.3405234376	0.0649766356
H	-0.3550704100	0.0993915968	0.9425828668

Frequencies (cm^{-1}):

1638.99 3888.28 3985.91

Rotational constants (GHz): 836.07048 433.64988 285.54466

RC- α [OH]:

Cartesian Coordinates (Å)

C	0.7212025027	-0.5316359814	-0.0658907980
O	0.9647711013	-1.7000888140	-0.1459261964
O	1.6930097212	0.4068311871	-0.0115075434
C	-0.6476202351	0.0913645338	-0.0143836074
C	-1.7516805148	-0.9523733842	-0.0736833350
H	-0.7168078380	0.8085636498	-0.8395922923
H	-0.7043034841	0.6986467343	0.8953551533
H	-1.6819884013	-1.5401588804	-0.9911557358
H	-1.6750447919	-1.6471432254	0.7650319325
H	-2.7275287448	-0.4656158813	-0.0403297947
C	3.0333171442	-0.0859819926	-0.0619987713
H	3.6695924200	0.7962192264	-0.0177401937
H	3.2273391800	-0.7465611489	0.7851380936
H	3.1997957961	-0.6365682479	-0.9898018795
O	0.6648425854	3.1303801597	0.3655910809
H	1.1295814494	2.2840197850	0.2313008172

Frequencies (cm^{-1}):

34.50 73.05 77.90 143.82 147.54 153.73 219.54 222.71 334.03 336.13 451.02
 524.87 578.91 676.99 814.12 873.51 1010.54 1051.31 1110.78
 1130.08 1181.08 1189.23 1233.47 1286.12 1394.45 1428.04 1446.35 1449.25
 1473.22 1484.38 1492.41 1497.84 1866.20 3064.34 3067.90 3069.58 3100.35
 3146.61 3154.67 3156.11 3182.52 3712.60
 Rotational constants (GHz): 2.44983 1.91575 1.09737

TS- α [OH]:

Cartesian Coordinates (Å)

C	0.7007290692	-0.4521313468	0.0335805126
O	0.9595627429	-1.4533258532	-0.5722488123
O	1.6391504896	0.4212473235	0.4401045064
C	-0.6755751157	-0.0055454627	0.4267561001
C	-1.7763712477	-0.8786427249	-0.1240557284
H	-0.7801399241	1.0935016350	-0.0030482504
H	-0.7201342641	0.1473411901	1.5085404240
H	-1.7123689366	-0.9409623326	-1.2120147963
H	-1.6791420835	-1.8963670945	0.2660463844
H	-2.7577648581	-0.4908636774	0.1527603231
C	2.9777860811	0.0571646961	0.1037489419
H	3.6168750554	0.8444579045	0.4999123385
H	3.2326463525	-0.9054522729	0.5522705709
H	3.0892093296	-0.0209762824	-0.9800135095
O	-0.4828091243	2.3856697832	-0.3988347734
H	0.4348042040	2.3741585047	-0.0859321417

Frequencies (cm^{-1}): 1023.78i

67.61 103.21 139.64 188.66 214.86 290.80 336.52 437.77 583.77 638.17 663.74
 838.92 872.34 925.64 1021.75 1064.17 1091.06 1138.08 1177.80 1208.10 1238.73
 1291.44 1355.68 1398.00 1459.02 1465.98 1468.70 1470.15 1486.93 1518.62
 1845.190 3043.15 3052.36 3092.25 3119.15 3134.34 3143.34 3168.95 3773.48

Rotational constants (GHz): 2.97984 1.94371 1.28485

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 293.57 -4.12 1.45 -295.14 -2.08 3.18 1.89 2.89 -46.52 2.32 2.74
 C1O2-C4H: 198.01 -0.89 -1.10 -184.69 0.81 0.93 -1.17 1.88 -6.42 1.72 -0.91

PC- α [OH]:

Cartesian Coordinates (Å)

C	0.7073116292	-0.6024159912	-0.1344162197
O	1.0835078840	-1.7302276826	-0.3532669734
O	1.5818115252	0.4280734327	0.0126820446
C	-0.6687420242	-0.1843269632	-0.0002438788
C	-1.7606863063	-1.1689973259	-0.1370994349
H	0.3298410571	3.0879003300	1.5258642773
H	-0.8688662541	0.8639379339	0.1912276261
H	-1.3590111059	-2.1668416448	-0.3191948890
H	-2.3836530806	-1.1918997223	0.7651654041

H	-2.4299231302	-0.8973786783	-0.9626075828
C	2.9523136340	0.0638122192	-0.1271863606
H	3.5274581848	0.9796460800	0.0023397982
H	3.2298691287	-0.6739590622	0.6292513196
H	3.1336473475	-0.3652037071	-1.1152260833
O	0.2355547892	2.9802038390	0.5799717531
H	0.8503470218	2.2802662427	0.3421614393

Frequencies (cm⁻¹):

40.28 84.14 96.55 114.07 139.88 157.98 180.84 189.18 221.54 238.14 353.49
 472.76 525.60 624.25 681.29 756.44 877.55 990.57 1028.30 1092.38
 1169.99 1181.90 1218.66 1231.01 1388.51 1432.99 1463.48 1465.98 1472.58
 1493.35 1513.26 1649.36 1765.45 3025.27 3061.92 3076.41 3143.58 3150.77
 3176.62 3215.01 3837.25 3955.76

Rotational constants (GHz): 2.36118 1.92542 1.07854

RC-β [OH]:

Cartesian Coordinates (Å)

C	-0.9615676316	-0.1412016012	0.006025278
O	-1.0244757066	1.0138303687	0.350038479
O	-2.0439894294	-0.8691647822	-0.250041578
C	0.3060345795	-0.9300434350	-0.183843436
C	1.5524464992	-0.1177030391	0.117470035
H	0.2299596780	-1.8169953856	0.454345921
H	1.6201580108	0.7539947332	-0.538639217
H	1.5434789829	0.2472981384	1.147762593
H	2.4549685294	-0.7150909896	-0.023338101
C	-3.2902822991	-0.1902768813	-0.089820718
H	-4.0644605348	-0.9301307879	-0.286294322
H	-3.3812387528	0.2026956636	0.925027463
H	-3.3636744816	0.6401296965	-0.795857956
H	0.3003050963	-1.3078277065	-1.211917782
O	1.1548815284	2.8173656404	0.891688544
H	0.3439403415	2.2942420481	0.737330268

Frequencies (cm⁻¹):

39.88 75.88 106.35 156.90 160.22 187.13 220.13 269.64 367.23 454.83 524.49
 549.37 586.36 668.22 813.06 895.35 1006.63 1047.71 1110.65 1117.70 1182.38
 1247.25 1272.40 1277.98 1395.79 1418.76 1454.60 1477.40
 1486.18 1489.56 1498.92 1524.54 1819.63 3056.51 3064.53 3066.91 3099.49
 3130.63 3142.34 3146.50 3186.83 3673.47

Rotational constants (GHz): 3.71422 1.45184 1.06455

TS-β [OH]:

Cartesian Coordinates (Å)

C	-0.8538488647	-0.1059753603	0.0819334964
O	-0.8724269283	0.9601561762	0.6419110396
O	-1.9602176160	-0.7328153493	-0.3148244501

C	0.3869906550	-0.8899541984	-0.2633096706
C	1.6309487843	-0.3124514565	0.3646239750
H	0.2182680496	-1.9295497317	0.0406053387
H	1.8003748055	0.7915665833	-0.0791864410
H	1.5494140119	-0.1772665978	1.4435007032
H	2.5373666329	-0.8563289441	0.0979361769
C	-3.1780487527	-0.0362344165	-0.0521528912
H	-3.9769741578	-0.6692787031	-0.4335586123
H	-3.2970378301	0.1294819424	1.0207838433
H	-3.1789249397	0.9313751772	-0.5587808834
H	0.4648032231	-0.9059487671	-1.3560234537
O	1.5728721641	2.0232788824	-0.5301431632
H	0.7359841529	2.1338274332	-0.0501871073

Frequencies (cm^{-1}): 1171.27i

68.50 140.25 156.59 212.88 342.63 354.40 430.63 457.43 578.88 650.38 739.76
 846.36 915.39 951.37 1010.46 1053.41 1102.06 1143.63 1206.50 1208.62 1243.64
 1263.12 1306.64 1399.99 1432.35 1445.40 1461.92 1470.48 1470.65 1485.93 1820.40
 3044.39 3053.19 3081.38 3090.70 3135.36 3166.68 3172.19 3743.21

Rotational constants (GHz): 4.52246 1.47122 1.22096

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

C2C1-O2C4: 2926.10 -1099.41 -1739.72 -120.45 31.95 -25.25 -76.08 -19.50 -23.25 -5.99
 4.65

C1O2-C4H: 204.42 1.60 2.71 -192.11 -2.44 -1.48 0.07 -0.04 1.90 0.01 0.10

PC- β [OH]:

Cartesian Coordinates ($\text{\AA}$)

C	0.4939815721	0.1592812746	0.2151213203
O	0.3759965854	-0.8101368556	0.9217606686
O	1.6516898257	0.5167722714	-0.3331005949
C	-0.6305404934	1.0819219278	-0.1809761997
C	-1.7505622012	1.0668038744	0.7902349775
H	-0.2237651722	2.0862444269	-0.3480090334
H	-2.7058135756	-1.3905868262	-0.2659073543
H	-1.7147809737	0.4111885240	1.6487819765
H	-2.6044476956	1.7113513507	0.6424152742
C	2.7462476504	-0.3586084947	-0.0603382378
H	3.6057266084	0.0618132048	-0.5789754606
H	2.9319815790	-0.4098985348	1.0145911823
H	2.5278473045	-1.3635372902	-0.4281408494
H	-0.9650718448	0.7256804358	-1.1691006321
O	-1.9139773065	-1.7814709801	-0.6348492801
H	-1.2606124725	-1.7243345889	0.0694636927

Frequencies (cm^{-1}):

33.63 101.72 113.63 148.98 163.81 173.21 182.02 192.91 237.51 263.88 357.14
 439.45 462.42 511.77 592.14 686.28 880.43 915.13 1020.34 1049.14
 1131.82 1182.72 1192.61 1214.57 1275.13 1403.09 1426.05 1450.01 1475.94

1478.25 1491.40 1651.39 1822.49 3001.15 3066.06 3066.77 3148.50 3185.68
3190.78 3303.87 3826.04 3947.00
Rotational constants (GHz): 3.52627 1.57149 1.26909

RC-m [OH]:

Cartesian Coordinates (Å)

C	0.5000685394	-0.1462066992	0.0472426457
O	0.1295179367	0.9678589928	-0.2321104938
O	-0.3186116085	-1.1896819808	0.1219918923
C	1.9280810568	-0.5137890909	0.3523469846
C	2.8572305413	0.6823028563	0.2351101376
H	1.9443993439	-0.9505400376	1.3566503654
H	2.8263498001	1.0976101439	-0.7742408769
H	2.5532780599	1.4753333547	0.9211207613
H	3.8876191546	0.4017203133	0.4627816586
C	-1.6945474679	-0.9086926982	-0.1440864859
H	-2.2309069378	-1.8476255971	-0.0180252577
H	-1.8197745120	-0.5278437989	-1.1601154943
H	2.2112732832	-1.3249458251	-0.3266435191
H	-2.0718900669	-0.1561711853	0.5523135676
O	-2.3460742502	2.1922193220	-1.0209349946
H	-1.4592743224	1.8776002501	-0.7561822808

Frequencies (cm⁻¹):

39.06 50.93 91.33 156.49 163.76 221.95 229.60 255.89 371.52 432.54 461.18
533.03 590.48 687.24 813.28 912.61 1008.82 1052.25 1113.58 1132.70 1171.30
1248.80 1276.89 1277.86 1410.73 1433.32 1454.21 1480.05
1482.31 1485.40 1499.43 1521.28 1822.18 3064.13 3065.52 3066.71 3101.93
3146.33 3146.81 3148.75 3187.04 3669.06

Rotational constants (GHz): 3.52285 1.43594 1.04004

TS-m [OH]:

Cartesian Coordinates (Å)

C	0.4580504567	-0.1704405870	-0.1071808484
O	0.1336473427	0.7954606315	-0.7448623729
O	-0.3899545163	-1.1720884621	0.1750889599
C	1.8249142031	-0.4191363325	0.4680270773
C	2.7885688981	0.7146025455	0.1609131725
H	1.7000595487	-0.5725074143	1.5451528786
H	2.8964826158	0.8497611825	-0.9171255569
H	2.4202525927	1.6567490766	0.5716586852
H	3.7724224410	0.5103404465	0.5868470756
C	-1.6880538103	-1.0368842251	-0.3420372182
H	-2.2606836331	-1.9132086498	-0.0443539609
H	-1.6857076094	-0.8605961119	-1.4193855613
H	2.1776471161	-1.3774648485	0.0721925075
H	-2.2135370158	-0.0821756312	0.1488569616

O -2.4637358991 1.1881048813 0.5252416705
 H -1.7482140209 1.5875701284 0.0049574999
 Frequencies (cm^{-1}): 1124.29i
 71.00 143.51 198.24 211.12 336.66 342.33 402.91 454.28 579.69 661.37 791.74
 808.52 895.87 916.18 1008.93 1071.07 1112.78 1128.68 1139.09 1238.45 1252.95
 1274.85 1358.25 1392.76 1409.43 1447.10 1455.93 1477.81 1485.79 1512.98 1829.17
 3051.06 3053.71 3083.03 3091.07 3134.51 3137.68 3184.44 3751.93
 Rotational constants (GHz): 4.46198 1.45740 1.22736
 V_i ($i = 0 - 10$) (cm^{-1}) for rotations:
 HC3-C2C1: 363.67 -1.03 0.78 -368.81 -1.72 0.87 1.79 0.78 0.03 2.80 1.57
 C3C2-C1O1: 354.70 -143.57 -64.00 -74.19 -7.29 1.42 -11.16 -64.00 6.36 -1.29 0.15

PC-m [OH]:

Cartesian Coordinates ($\text{\AA}$)

C 0.3905877038 -0.2404222134 -0.3690147495
 O 0.2006457047 0.4767303454 -1.3099361869
 O -0.5011325087 -1.1952924609 0.0103819876
 C 1.5722790090 -0.2102532312 0.5521666318
 C 2.6484653392 0.7457215271 0.0665939299
 H 1.1758862701 0.0900240413 1.5292138149
 H 3.0173567867 0.4516653335 -0.9184826870
 H 2.2491496695 1.7579106515 -0.0210097514
 H 3.4899626961 0.7634023244 0.7614069403
 C -1.6855140741 -1.2476154565 -0.6498182187
 H -2.3096256769 -2.0777147485 -0.3632730735
 H -1.7875720823 -0.6765894963 -1.5599843449
 H 1.9417269289 -1.2338051959 0.6695747245
 H -1.9477199298 0.9395678569 1.0782973509
 O -1.2461343992 1.5920961385 1.1026873875
 H -1.1065277068 1.8359964639 0.1853415047

Frequencies (cm^{-1}):

36.38 76.02 92.46 141.69 160.13 169.28 217.37 220.51 255.69 302.31 365.15
 376.64 464.33 480.79 574.35 667.93 810.50 859.09 1015.88 1090.93
 1109.62 1160.56 1202.27 1268.85 1281.17 1391.42 1412.39 1447.45 1453.85
 1484.25 1491.21 1643.78 1850.25 3061.03 3064.69 3104.17 3144.81 3150.65
 3200.09 3352.48 3861.73 3951.03

Rotational constants (GHz): 3.06698 1.81084 1.45384

HO₂ + CH₃CH₂C(=O)OCH₃ → Products

HO₂:

Cartesian Coordinates ($\text{\AA}$)

O -0.0507331544 0.1160170748 -0.1074187288
 H 0.0528333232 -0.1208197614 0.8261903324
 O 0.3960390112 -0.9056658935 -0.7877696636

Frequencies (cm^{-1}):

1247.13 1465.26 3738.77

Rotational constants (GHz): 633.65106 34.76897 32.96041

H₂O₂:

Cartesian Coordinates (Å)

O	-0.0777932178	0.0111396546	-0.0300181604
H	-0.0305586801	-0.0081576077	0.9296746240
O	1.2841959957	0.2490526408	-0.3717170463
H	1.2327759422	1.1326367224	-0.7462152572

Frequencies (cm⁻¹):

384.51 1029.94 1361.70 1472.52 3866.26 3868.56

Rotational constants (GHz): 308.53718 27.30221 26.43930

RC- α [HO₂]:

Cartesian Coordinates (Å)

C	-0.5858854648	0.4392630499	0.1840073787
O	-0.6231264575	0.5367261084	-1.0249741080
O	-1.4538312501	-0.2913534924	0.8665670795
C	0.4033892054	1.1386675428	1.0729008283
C	1.5127552610	1.8068094599	0.2781359942
H	0.7914192739	0.3914942593	1.7710314643
H	-0.1571933684	1.8613279080	1.6768937465
H	2.0831445699	1.0624762468	-0.2836862307
H	1.1028856338	2.5236669623	-0.4361689603
H	2.2007609766	2.3314819707	0.9432731628
C	-2.3605617936	-1.0591058009	0.0757364297
H	-2.9961410202	-1.5942879748	0.7785347211
H	-2.9564534149	-0.4072936966	-0.5663057829
H	-1.8017947371	-1.7628677422	-0.5470872642
O	1.2325119460	-1.5576199893	-0.4115292937
O	1.2582229813	-1.2339428869	-1.6728172611
H	0.6083218088	-0.4983888151	-1.7515019140

Frequencies (cm⁻¹):

35.14 75.53 81.51 95.76 159.83 182.16 207.15 227.05 247.79 290.00 352.91 458.54
582.40 590.63 672.61 813.79 891.42 1008.87 1051.04 1113.28 1121.68 1181.40
1214.96 1276.22 1281.57 1283.52 1401.41 1415.76 1447.75 1477.12 1478.06
1485.36 1488.20 1497.40 1548.45 1787.95 3060.65 3061.00 3064.76 3110.55
3142.79 3144.11 3150.05 3185.72 3480.77

Rotational constants (GHz): 2.05175 1.73709 1.16433

TS- α [HO₂]:

Cartesian Coordinates (Å)

C	-0.6447982696	0.2431124798	0.0473087449
O	-0.6271157142	0.0598080903	-1.1502630266
O	-1.6516223129	-0.1518605088	0.8251239195
C	0.4692634925	0.8498315621	0.8062325819
C	1.2638060684	1.9094136823	0.1071581409

H	1.2857203009	-0.2499012892	0.7191353896
H	0.2828881709	0.9600644682	1.8717704403
H	1.5652238543	1.5666531236	-0.8857738121
H	0.6636639021	2.8184849933	-0.0249665042
H	2.1557223835	2.1713283582	0.6783017352
C	-2.7027251203	-0.8402024061	0.1487288204
H	-3.4397127559	-1.0890277965	0.9099721288
H	-3.1430522596	-0.2015376878	-0.6201077297
H	-2.3180657622	-1.7463353226	-0.3248888776
O	1.8016468551	-1.1993064453	0.2630430243
O	2.1010494303	-0.8411046766	-1.0305334176
H	1.2482694768	-0.9084000546	-1.4878725878

Frequencies (cm^{-1}): 2230.76i

99.06 137.64 160.02 190.63 219.89 298.02 348.39 457.52 519.02 545.32 674.40
 742.78 857.40 886.86 1016.75 1035.30 1067.48 1074.81 1125.94 1165.17 1204.60
 1207.55 1255.26 1383.27 1409.95 1457.47 1460.38 1462.68 1470.06 1477.06 1483.77
 1485.46 1766.59 3020.20 3052.93 3099.31 3135.18 3138.69 3166.23 3173.23 3719.09

Rotational constants (GHz): 2.82738 1.30603 1.11222

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 166.29 -3.77 -0.44 -173.39 0.86 3.98 0.13 -0.44 -24.10 2.71 0.43 C2C1-
 O2C4: 2858.87 -1119.63 -792.60 -148.70 8.77 0.03 -206.71 -792.60 -53.19 24.85 9.60
 C1O2-C4H: 205.40 0.13 -0.95 -193.34 1.35 -0.07 -1.70 -0.95 -5.90 2.69 -1.97

PC- α [HO₂]:

Cartesian Coordinates (Å)

C	-0.7539265350	0.3921409538	0.1467383155
O	-0.5371661338	-0.0168451075	-0.9802697763
O	-1.8257780650	0.0127831720	0.8501115956
C	0.0783292579	1.3304408948	0.8634113616
C	1.2944889319	1.9003891691	0.2500152399
H	2.7437537912	-0.6760117231	0.4717509853
H	-0.2343820666	1.6107564039	1.8610561519
H	1.5401892922	1.3868496573	-0.6814731774
H	1.1591237627	2.9677750310	0.0300723308
H	2.1456175809	1.8363553134	0.9371604985
C	-2.6658002887	-0.9357875332	0.1986881203
H	-3.4767448733	-1.1487256350	0.8929802173
H	-3.0569358984	-0.5226795605	-0.7341340596
H	-2.1055479319	-1.8457386773	-0.0290000560
O	1.9721548810	-1.2185169552	0.2902667475
O	1.9640441375	-1.2139871153	-1.1369266205
H	1.0959313373	-0.8121295681	-1.3027518646

Frequencies (cm^{-1}):

37.76 68.93 87.73 119.25 145.36 162.65 167.92 206.87 211.15 225.61 242.16
 360.41 474.11 580.18 602.00 684.33 754.33 889.58 989.04 1026.22 1030.83
 1085.53 1167.18 1181.66 1215.35 1262.14 1365.80 1391.81 1434.77 1462.03

1468.33 1474.91 1490.32 1514.95 1540.63 1741.38 3020.76 3061.65 3075.40
3141.90 3147.48 3181.85 3232.40 3705.60 3871.97
Rotational constants (GHz): 2.44755 1.29059 0.99703

RC- β [HO₂]:

Cartesian Coordinates (Å)

C	0.6557363456	-0.0300327940	-0.2803432380
O	0.4931547973	-1.2246544330	-0.1564518481
O	1.7949831320	0.5581427769	0.0592505956
C	-0.3721051388	0.9459510087	-0.7737793216
C	-1.0112044763	1.6757373385	0.4128786650
H	0.1189301976	1.6590337690	-1.4408902028
H	-1.5225569259	0.9605058382	1.0605049876
H	-0.2554558321	2.2119806098	0.9916397754
H	-1.7478936735	2.3974041803	0.0562438549
C	2.7984822240	-0.3046393629	0.5977888210
H	3.6499290812	0.3320094965	0.8298593050
H	2.4288498563	-0.7988366168	1.4986314212
H	3.0748042993	-1.0663149050	-0.1342991179
H	-1.1288300175	0.3895862897	-1.3288072119
O	-2.6538810507	-1.2175590634	0.0338084682
O	-1.9965747097	-2.2476843651	-0.4248448613
H	-1.0481904687	-1.9886134373	-0.3670683825

Frequencies (cm⁻¹):

18.87 50.40 97.54 109.49 129.66 139.77 170.05 215.84 224.31 278.69 337.31
449.91 634.85 665.39 769.37 803.92 893.00 983.61 1051.40 1099.37
1128.05 1182.09 1216.59 1259.00 1282.65 1326.23 1371.03 1399.39 1467.08
1476.39 1477.18 1489.74 1492.32 1500.63 1578.21 1799.17 3059.46 3067.46
3084.36 3138.47 3150.32 3150.65 3157.73 3187.97 3458.82

Rotational constants (GHz): 2.78664 1.15037 0.87934

TS- β [HO₂]:

Cartesian Coordinates (Å)

C	-0.6440353184	-0.1229201113	-0.5109793128
O	-0.5856002840	1.0604436571	-0.7348641865
O	-1.6692461598	-0.6880452879	0.1189605451
C	0.4227676405	-1.1295451385	-0.8693065380
C	1.1669538758	-1.5756648846	0.3617795641
H	-0.0600853761	-1.9881059605	-1.3547780080
H	1.6903284339	-0.3770065249	0.8396881875
H	0.5508375932	-1.9142878561	1.1923467570
H	2.0560180719	-2.1754025645	0.1843572808
C	-2.6874527873	0.2157963183	0.5534753688
H	-3.4348718804	-0.3921157720	1.0593194512
H	-2.2656762022	0.9576332845	1.2346987824
H	-3.1254141318	0.7317630513	-0.3034046978

H	1.1029725264	-0.6620066678	-1.5841116501
O	1.9353240796	0.7189489701	1.0438419144
O	2.1877202887	1.2574658429	-0.2100065662
H	1.3091985500	1.5561162037	-0.4937897617

Frequencies (cm^{-1}): 2400.10i

70.97 135.82 150.86 183.58 233.20 303.73 321.23 428.68 471.92 579.09 629.13
 659.12 747.75 834.79 881.63 984.85 1032.16 1052.89 1057.69 1113.34 1148.39
 1204.51 1207.44 1216.85 1325.85 1354.28 1436.00 1444.81 1469.46 1470.23 1472.39
 1485.12 1496.87 1814.71 3024.94 3055.85 3107.65 3117.97 3139.94 3175.78 3207.95
 3705.75

Rotational constants (GHz): 2.95868 1.28621 1.10735

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

C1O2-C4H: 210.08 -0.95 -1.25 -197.65 1.35 0.72 1.28 -2.34 -11.09 -1.98 1.33

C2C1-O2C4: 3097.10 -1305.41 -1744.53 -64.70 42.38 -19.59 137.81 178.87 22.73 1.93 -
 57.18

PC- β [HO_2]:

Cartesian Coordinates ($\text{\AA}$)

C	-0.5087569784	-0.1817262805	-0.6322791456
O	-0.5458102631	0.9054991653	-1.1530181736
O	-1.3398764461	-0.5572874755	0.3301373534
C	0.4691493554	-1.2671545252	-1.0223207503
C	0.9782968844	-2.0789294817	0.1129912161
H	-0.0574191233	-1.9051868147	-1.7535706005
H	1.6668180589	-0.0159411388	1.1869710726
H	0.3431477351	-2.2776201633	0.9648837384
H	1.8984629729	-2.6349919302	0.0010787032
C	-2.1923624260	0.4792811491	0.8217129285
H	-2.7979153419	0.0263946133	1.6044777130
H	-1.5796779954	1.2899302111	1.2240631147
H	-2.8231111190	0.8669149587	0.0194698076
H	1.2787047298	-0.7816493775	-1.5740717000
O	1.3047150486	0.8781749147	1.1875120364
O	1.9595540745	1.4571040540	0.0618927821
H	1.2104140934	1.5835186812	-0.5390984261

Frequencies (cm^{-1}):

53.05 60.41 101.98 122.22 153.86 174.86 188.00 197.69 212.16 256.22 336.07
 345.88 460.70 548.95 571.55 613.51 666.34 867.26 920.50 982.67
 1026.37 1085.04 1127.12 1183.43 1192.74 1218.47 1334.38 1361.63 1385.09
 1430.62 1452.57 1475.15 1476.93 1488.82 1516.84 1819.35 2975.63 3064.82
 3105.90 3150.51 3185.76 3186.36 3298.54 3747.92 3798.97

Rotational constants (GHz): 2.10432 1.64520 1.29427

RC-m [HO_2]:

Cartesian Coordinates ($\text{\AA}$)

C	-2.3481329633	0.3773522410	-0.2952307173
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C	-0.8795524663	0.3219953536	0.0266684695
O	-0.2937446929	-0.6850583856	0.3527728735
O	-0.2930395877	1.5034423139	-0.0835100649
C	1.1112459207	1.5346921414	0.1911593307
H	-2.4408261827	0.7772897066	-1.3105899829
H	-2.7962097369	1.1316646185	0.3599504966
H	1.4182702499	2.5705272856	0.0629494225
H	1.6516494484	0.8823873526	-0.4986953908
H	1.3041479339	1.2068983152	1.2162635533
O	2.9679573944	-1.1192008575	-0.1371082247
O	2.2552181357	-1.5470265602	0.8692829930
H	1.3377815001	-1.2410516809	0.6979398203
C	-3.0223039997	-0.9768304057	-0.1526026924
H	-2.5626062642	-1.7104182548	-0.8177256155
H	-4.0840470137	-0.9047186850	-0.3945980474
H	-2.9230709357	-1.3541607486	0.8670959262

Frequencies (cm^{-1}):

30.55 46.59 67.86 92.82 129.19 160.79 193.88 223.88 233.18 250.30 357.30
 459.15 584.71 601.60 674.00 812.40 893.86 1004.96 1046.20 1113.98 1121.33
 1178.13 1218.99 1279.07 1281.05 1282.82 1404.23 1417.41 1452.52 1479.20
 1484.19 1485.36 1495.52 1496.67 1562.93 1806.70 3060.31 3064.31 3067.09
 3102.77 3146.11 3147.83 3151.24 3188.81 3524.12

Rotational constants (GHz): 3.03161 0.99199 0.78185

TS-m [HO_2]:

Cartesian Coordinates ($\text{\AA}$)

C	-2.2887797845	0.3251714836	-0.3986132475
C	-0.8876595334	0.2865167158	0.1418593816
O	-0.3962009335	-0.6280234756	0.7451437132
O	-0.2212107283	1.4264504368	-0.1297211496
C	1.0753684577	1.5235156401	0.3497869583
H	-2.2147717739	0.5295086758	-1.4720778073
H	-2.7837113605	1.2009402266	0.0347107690
H	1.4821428730	2.5025712912	0.1178457325
H	1.8247710423	0.5734957188	-0.2964582663
H	1.2084564718	1.1511120853	1.3668960783
O	2.2535169316	-0.4397445738	-0.6478236763
O	2.4012572372	-1.1497451272	0.5324058452
H	1.4953488431	-1.4326914130	0.7207397298
C	-3.0467527394	-0.9599667010	-0.1124371218
H	-2.5382585961	-1.8163561614	-0.5598318046
H	-4.0594369834	-0.9069482131	-0.5157988041
H	-3.1089704137	-1.1419185387	0.9623914798

Frequencies (cm^{-1}): 2352.07i

60.74 128.99 141.90 180.46 207.46 237.40 348.57 454.54 522.94 569.58 583.22
 622.24 671.58 806.53 872.74 1010.27 1049.69 1061.99 1080.88 1112.91 1138.10

1205.41 1213.41 1248.62 1274.51 1388.25 1409.24 1445.63 1453.18 1470.56 1478.29
1484.47 1486.91 1830.86 3050.59 3053.52 3085.62 3090.28 3134.25 3138.32 3222.85
3756.39

Rotational constants (GHz): 3.35761 1.10210 0.91478

V_i ($i = 0 - 10$) (cm^{-1}) for rotations:

HC3-C2C1: 373.29 -0.94 0.65 -377.47 -1.41 0.84 1.48 0.65 -1.24 2.67 1.40

C3C2-C1O1: 367.60 -147.05 -64.00 -80.77 -9.48 1.78 9.43 -64.00 -3.43 1.91 0.11

PC-m [HO₂]:

Cartesian Coordinates (Å)

C -1.9800066409 0.1762188731 -0.4826615794
C -0.7807500050 0.3526747305 0.3978185226
O -0.4410251264 -0.3808421433 1.2873154884
O -0.0885562476 1.4714872550 0.0740390199
C 1.1083599408 1.6764051162 0.6819174381
H -1.5934814832 0.0669449179 -1.5024058005
H -2.5498827370 1.1110069724 -0.4705086174
H 1.5543852816 2.6315866379 0.4620172182
H 1.7466295729 -0.2531854427 -1.2011142707
H 1.3941461847 1.0203428824 1.4893858190
O 1.1187775860 -0.9814114011 -1.1557368956
O 1.6322744614 -1.7368899722 -0.0640757792
H 1.0021616208 -1.5052833769 0.6337742499
C -2.8177773198 -1.0215467653 -0.0693978217
H -2.2222716879 -1.9357118090 -0.1088571984
H -3.6763970812 -1.1369123231 -0.7329234534
H -3.1814709392 -0.9089092320 0.9541792598

Frequencies (cm^{-1}):

22.17 51.70 78.93 112.20 152.26 172.47 199.76 221.02 233.94 284.56 301.64
369.57 413.12 466.14 546.82 572.41 666.61 808.52 862.89 1015.77
1027.43 1091.87 1109.10 1163.35 1200.44 1273.60 1279.85 1391.69 1395.51
1413.61 1445.51 1456.45 1484.32 1492.01 1500.91 1831.88 3061.44 3065.29
3102.29 3146.05 3151.91 3204.87 3359.04 3753.37 3841.01

Rotational constants (GHz): 2.18909 1.53786 1.13356

Table S2: Optimized geometries of the distinct conformers of MP and their energies (in kcal/mol) relative to the most stable conformation obtained using DFT-M08-HX/cc-pVTZ; the mirror image structure has the same relative energy as its corresponding conformer.

Relative energy	Mirror image	Cartesian Coordinates (Å)
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0.0	No	C	0.1972813350	1.4159020169	-0.5146224137
		C	-0.0002383758	0.0003064767	0.0007442885
		C	1.2082833832	-0.5013045063	0.7489755581
		O	2.2184149915	0.1196756238	0.9337956045
		O	1.0271901722	-1.7505822262	1.1978480777
		C	2.1311056586	-2.2920891717	1.9180283132
		H	1.0558915599	1.4654126217	-1.1873608780
		H	-0.6880813895	1.7602083137	-1.0525377983
		H	0.3937976926	2.1032190678	0.3107497300
		H	-0.8588242061	-0.0738343774	0.6764789729
		H	-0.2012291513	-0.7070710792	-0.8107074679
		H	2.3485097362	-1.6830338558	2.7986758413
		H	3.0224316989	-2.3203008724	1.2868193829
		H	1.8389428945	-3.2988030317	2.2123017885
1.3	Yes	C	-1.2580158097	-0.0625754584	0.8518973237
		C	0.0203086967	0.0659981630	0.0285961578
		C	1.2435776503	-0.4980609567	0.7075470803
		O	2.3354987089	-0.0007118206	0.6905840523
		O	0.9840342310	-1.6564802991	1.3303416770
		C	2.1085613200	-2.2571483591	1.9663489443
		H	-1.1617860417	0.4559768247	1.8091851008
		H	-2.1027069930	0.3739251830	0.3151018261
		H	-1.4838074686	-1.1098442935	1.0588676201
		H	-0.0893486228	-0.4714451384	-0.9206898194
		H	0.2487946208	1.1047858258	-0.2151014534
		H	2.5220041787	-1.5865777379	2.7231761562
		H	2.8889610309	-2.4768760651	1.2339303990
		H	1.7450134987	-3.1751038679	2.4253629352
7.1	Yes	C	-0.9556088726	2.0151872168	-1.2789369920
		C	-1.2601473517	0.6007185836	-0.8141808336
		C	-0.0943419998	0.0127896682	-0.0474848380
		O	0.9247511461	0.6032160555	0.1537171976
		O	-0.2278686236	-1.2425846594	0.4265699134
		C	-1.4229601964	-1.9702513329	0.2065403034
		H	-0.0738666540	2.0256090173	-1.9221541341
		H	-1.8001975264	2.4317857192	-1.8312570603
		H	-0.7386811536	2.6603718913	-0.4257260073
		H	-2.1490599157	0.5761025948	-0.1733632586
		H	-1.4881271518	-0.0549028509	-1.6626606887
		H	-1.6139448569	-2.1246939388	-0.8600176284
		H	-2.2877852069	-1.4791216046	0.6634954890
		H	-1.2774526368	-2.9398553602	0.6817745374
9.5	Yes	C	-2.4837306683	0.9854624287	0.1719074829
		C	-1.3645112144	0.4815323775	-0.7468890555
		C	-0.2114420838	-0.0244942547	0.0936659485
		O	0.6702816394	0.6892669126	0.4696239407

	O	-0.2190232805	-1.3147753789	0.4869205167
	C	-1.2025827727	-2.2133595262	0.0043833525
	H	-2.0994824771	1.7670098933	0.8311049392
	H	-3.3068191431	1.3997702957	-0.4133237796
	H	-2.8835407781	0.1845830001	0.8003337497
	H	-1.7398906643	-0.2785198311	-1.4353871920
	H	-0.9692123281	1.3094706072	-1.3367578596
	H	-1.0814407011	-2.4002687880	-1.0674091387
	H	-2.2179024242	-1.8555138059	0.2003172585
	H	-1.0483811038	-3.1476359303	0.5437858370

Table S3: Optimized geometries of the distinct conformers of the transition states (TSs) for MP H-abstraction by OH and their energies (in kcal/mol) relative to the most stable conformation obtained using DFT-M08-HX/cc-pVTZ; the mirror image structure has the same relative energy as its corresponding conformer. The conformers with energies highlighted in bold are used in the semi-MS calculations.

TS- <i>a</i> [OH]				
Relative energy	Mirror image	Cartesian Coordinates (Å)		
0.00	Yes	C	-0.0000082023	-0.0002532243 0.0000897459
		O	0.2587090730	-1.0010991988 -0.6064154614
		O	0.9384463341	0.8727910712 0.4072389466
		C	-1.3762822602	0.4464736660 0.3931992519
		C	-2.4771804670	-0.4264810200 -0.1575746650
		H	-1.4805645305	1.5453714693 -0.0370156507
		H	-1.4209024837	0.5996443589 1.4749301127
		H	-2.4125177328	-0.4897362631 -1.2454392106
		H	-2.3808560046	-1.4439310756 0.2334605275
		H	-3.4585300470	-0.0378825727 0.1182654411
		C	2.2770210982	0.5093320948 0.0700280122
		H	2.9159793510	1.2970458795 0.4655393456
		H	2.5327814626	-0.4530303103 0.5185694810
		H	2.3876902102	0.4309717601 -1.0137838660
		O	-1.1829742615	2.8375700969 -0.4328524096
		H	-0.2660185394	2.8265892681 -0.1179546013
0.17	Yes	C	0.0160853420	0.2859270637 -0.2701877669
		O	0.9238243218	1.0419870076 -0.0326631411
		O	0.1350628653	-0.7501725277 -1.0991816109

		C	-1.3552390037	0.4027603128	0.3328929789
		C	-2.4866802892	-0.2688055221	-0.4093428495
		H	-1.5403843777	1.5880568744	0.3853723535
		H	-1.2963253840	0.1250122004	1.3890907895
		H	-2.5468763880	0.0868297716	-1.4401045034
		H	-2.3339741583	-1.3518782681	-0.4407380442
		H	-3.4401714276	-0.0695482801	0.0825538369
		C	1.4253356107	-0.9026270688	-1.6912507252
		H	1.3600213682	-1.7752769178	-2.3384084874
		H	1.6839086123	-0.0120388180	-2.2680212532
		H	2.1820286007	-1.0510217900	-0.9178497234
		O	-1.2740199102	2.8976055858	0.4468566878
		H	-0.3082807822	2.7894283764	0.4381274584
7.82	Yes	C	-0.1458598702	-0.0701795631	0.0872811695
		O	0.5098443752	0.4942915161	-0.7444213619
		O	0.3361692208	-1.1882376017	0.6468299702
		C	-1.5204702079	0.4058840300	0.4868688914
		C	-2.5927987906	-0.0957239377	-0.4648468267
		H	-1.4692301171	1.6025321261	0.3383942838
		H	-1.7591411316	0.2524771077	1.5404795765
		H	-2.3335423823	0.1809266932	-1.4893072190
		H	-2.6953734283	-1.1860808538	-0.4217518099
		H	-3.5595261638	0.3471086235	-0.2204497981
		C	-0.4147756299	-1.8778435824	1.6357788070
		H	0.1136040057	-2.8133192280	1.8152819476
		H	-0.4580118697	-1.3084602097	2.5689746209
		H	-1.4290363640	-2.1011790896	1.2925269549
		O	-1.1854142462	2.7501480738	-0.2410323331
		H	-0.4280074000	2.4019538956	-0.7420958730
1.31	Yes	C	1.4146829719	-0.5265537782	-0.3188868829
		O	2.2440194919	-1.0067998282	0.3999678235
		O	1.5914711171	-0.3869134853	-1.6465064174
		C	0.0719145138	-0.0159680902	0.1105919150
		C	-1.0971620302	-0.7574285713	-0.5106639685
		H	0.0166053613	1.1035068115	-0.2752569865
		H	0.0371939480	0.0374931287	1.1990552475
		H	-1.0304362973	-0.7353331599	-1.6004266822
		H	-1.1113081989	-1.8028698375	-0.1863036607
		H	-2.0405110238	-0.2963768632	-0.2137968612
		C	2.8426089706	-0.8690810334	-2.1360385911
		H	2.8359793384	-0.6989667135	-3.2113452234
		H	3.6673297265	-0.3293858323	-1.6653188441
		H	2.9499051797	-1.9334481366	-1.9163869187
		O	0.0354040542	2.1458200009	-1.1830656379
		H	0.5292048767	1.6694973887	-1.8684983114
0.56	Yes	C	1.3989489541	0.0555626580	-0.5379196523

		O	1.6060132736	-0.0066960365	-1.7240992840
		O	2.3589517890	-0.0582728975	0.3768187593
		C	0.0380166284	0.2674663184	0.0549381466
		C	-0.9250751054	-0.8551207304	-0.2779427632
		H	-0.3642614225	1.2369538536	-0.5220905732
		H	0.0847078142	0.5273725830	1.1128997180
		H	-0.9274074119	-1.0360042913	-1.3551407922
		H	-0.6376684665	-1.7820479076	0.2289619850
		H	-1.9381599543	-0.5958426139	0.0332760916
		C	3.6717310993	-0.2553197091	-0.1501688240
		H	4.3354639214	-0.3247631550	0.7095082380
		H	3.7089632490	-1.1724161816	-0.7420156008
		H	3.9524403987	0.5854590010	-0.7881863005
		O	-0.6170887721	1.9700371523	-1.6309521053
		H	0.0009280047	1.4889889563	-2.2065550431
7.33	Yes	C	1.3625751012	-0.4231351912	-0.3088376841
		O	1.6047888332	-1.4408765715	-0.8886182753
		O	2.3649883386	0.3226233203	0.1766745849
		C	-0.0520555290	0.0678383751	-0.0987531718
		C	-1.0864692767	-0.8899142689	-0.6417027757
		H	-0.1161087823	1.0821415619	-0.6815256849
		H	-0.2228526401	0.3460566759	0.9454105948
		H	-0.9076127261	-1.0863001873	-1.6999351378
		H	-1.0227567503	-1.8489404584	-0.1202825275
		H	-2.0957852633	-0.4925757423	-0.5147456890
		C	2.0903356145	1.5213762744	0.8904493355
		H	3.0570821025	1.9927631982	1.0630533738
		H	1.4541328886	2.2001527834	0.3165569670
		H	1.6270339146	1.3045935910	1.8587673522
		O	-0.4176045913	2.3626238103	-1.2403911428
		H	-1.3504132340	2.4108998292	-0.9834441192
9.09	Yes	C	1.2991518200	-0.3160226182	-0.3433142353
		O	1.5575898638	-1.2675237180	-1.0228272521
		O	2.2945657509	0.4461504949	0.1332673711
		C	-0.1191576072	0.0872520657	-0.0221937035
		C	-1.1404407661	-0.9172443616	-0.4998401795
		H	-0.2913258475	1.1073695923	-0.5757452767
		H	-0.2383268217	0.3647792684	1.0290151446
		H	-1.0082590764	-1.1258559087	-1.5627774978
		H	-1.0126699044	-1.8656639882	0.0302204253
		H	-2.1545768649	-0.5532924121	-0.3268951470
		C	2.0109583271	1.5868956671	0.9339407404
		H	2.9694107979	2.0762950779	1.1029470676
		H	1.3373653852	2.2779375800	0.4204877790
		H	1.5895998748	1.2964615714	1.9016532617
		O	-0.2464330553	2.2180375909	-1.4715048369

		H	0.1317201238	1.7591440981	-2.2374556608
9.62	Yes	C	1.2740222533	-0.8869425745	-0.5478943571
		O	1.9509744977	-1.5220040498	0.2071135839
		O	1.4541981560	-1.0065718599	-1.8684229402
		C	0.1467618278	-0.0188099261	-0.0304421320
		C	-1.1883648358	-0.7482936236	-0.0523835989
		H	0.0310398179	0.9634043983	-0.6661377413
		H	0.4161154448	0.2989157554	0.9775850353
		H	-1.4451556392	-1.0956376217	-1.0561889313
		H	-1.1426166322	-1.6224238887	0.6039817134
		H	-1.9881822766	-0.0927068149	0.2966431531
		C	0.7899252867	-0.1286478554	-2.7714987857
		H	1.0120162070	-0.5059685103	-3.7687361836
		H	-0.2932255006	-0.1252523900	-2.6211600658
		H	1.1637553755	0.8929525842	-2.6724248851
		O	-0.4011581513	2.2118152647	-1.1563624370
		H	-0.3468468314	2.7156621125	-0.3315994279
TS- β [OH]					
Relative energy	Mirror image	Cartesian Coordinates (Å)			
0.0	Yes	C	0.0001051412	0.0000652841	0.0005359406
		O	-0.0186220963	1.0653736811	0.5620709458
		O	-1.1060917632	-0.6258743320	-0.3980402751
		C	1.2408359928	-0.7841954007	-0.3444430760
		C	2.4848760672	-0.2064061573	0.2828797910
		H	1.0719643873	-1.8234907272	-0.0395708299
		H	2.6536130667	0.8975456685	-0.1609964507
		H	2.4041174051	-0.0716074690	1.3618618417
		H	3.3913214320	-0.7498440444	0.0153658790
		C	-2.3241178955	0.0699916868	-0.1344467929
		H	-3.1228785885	-0.5625571070	-0.5172371933
		H	-2.4433885004	0.2337087647	0.9388285424
		H	-2.3250727126	1.0385658278	-0.6393519644
		H	1.3184363732	-0.8012334468	-1.4371329266
		O	2.4259647796	2.1284807254	-0.6146787668
		H	1.5900639111	2.2409670458	-0.1334526649
2.8	Yes	C	-2.4719266768	-0.4989875059	0.0543215453
		O	-3.2613667227	-1.1941241076	0.6264814471
		O	-2.8288328096	0.6493941647	-0.5515083291
		C	-1.0006019185	-0.7983455460	-0.0927487176
		C	-0.0931219390	0.4132791615	-0.0348067572
		H	-0.7578759937	-1.5245910701	0.6874066349
		H	-0.1774851651	1.0187281850	-1.0579310679
		H	-0.3471568150	1.1205010939	0.7561985814
		H	0.9613252136	0.1383498225	0.0123113765
		C	-4.2167087956	0.9722909176	-0.4468636350

		H	-4.3480387152	1.9232214854	-0.9606342155
		H	-4.8234350027	0.1936522470	-0.9138802950
		H	-4.5051832119	1.0594952969	0.6025356441
		H	-0.8708135898	-1.3102962234	-1.0540608353
		O	-0.5768563305	1.4593076404	-2.2724311742
		H	-1.5215095276	1.4186134381	-2.0600982024
3.4	Yes	C	-1.2786535852	0.7462801083	0.3698492881
		O	-1.2476992113	1.8012176665	0.9412270529
		O	-2.4105128248	0.1753586237	-0.0558457383
		C	-0.0727077841	-0.0991820334	0.0374794549
		C	1.2047619491	0.5278860669	0.5421169942
		H	-0.2313752327	-1.0947347876	0.4631042649
		H	2.0945775327	-0.1892416270	0.2344366416
		H	1.4024515609	1.5055568902	0.1012577444
		H	1.2552923502	0.5944352208	1.6298895975
		C	-3.5959272955	0.9177410683	0.2218488363
		H	-4.4214854093	0.3346015856	-0.1824979309
		H	-3.7151297965	1.0565961476	1.2988621608
		H	-3.5506086694	1.9004345854	-0.2532021606
		H	-0.0509169441	-0.2400656866	-1.0479271835
		O	3.0211273587	-0.9668085572	-0.4211042092
		H	3.3609050012	-0.2811682713	-1.0137948131
3.8	Yes	C	-2.4993104194	0.2595654776	-0.3495669858
		O	-2.5098462591	1.4112508845	-0.0152602282
		O	-3.6090189974	-0.4421761783	-0.6024327423
		C	-1.2575121167	-0.5702653053	-0.5680174579
		C	-0.0372284874	0.0764851370	0.0404026109
		H	-1.4326961327	-1.5705725648	-0.1630864618
		H	-0.1609047390	0.0127039392	1.2127431386
		H	0.8906496738	-0.4369901679	-0.2125446641
		H	0.0268133291	1.1456730242	-0.1672383231
		C	-4.8242742151	0.2866626225	-0.4447485833
		H	-5.6287187442	-0.4092893054	-0.6765183103
		H	-4.9165648839	0.6537766331	0.5798772432
		H	-4.8478456054	1.1413284083	-1.1249708477
		H	-1.1427065435	-0.6929036016	-1.6529287096
		O	-0.3558901563	-0.5176734191	2.4839327320
		H	0.4266582972	-1.0867745840	2.5053215894
4.5	Yes	C	-1.3375464905	0.6513699002	0.4927651980
		O	-2.0574338187	0.8753598417	-0.4392724117
		O	-1.5042516676	1.2144801126	1.6966069224
		C	-0.1575290169	-0.2934302070	0.4765091572
		C	1.0921358979	0.3099088755	1.0863504866
		H	-0.4473904641	-1.1868101895	1.0400982833
		H	1.9293226016	-0.5212886814	1.0835321781
		H	1.4855025226	1.1566146364	0.5204931929

		H	0.9713499384	0.5764728034	2.1370270138
		C	-2.6165811142	2.1012926844	1.7928612405
		H	-2.6178218527	2.4783982024	2.8140926976
		H	-2.5117772545	2.9219510996	1.0796132685
		H	-3.5466665226	1.5701117439	1.5781535327
		H	-0.0015713749	-0.5923510827	-0.5606033443
		O	2.8141541954	-1.5470824830	0.7926618034
		H	3.1152864209	-1.2162622565	-0.0658192192
4.6	Yes	C	-2.5420619904	0.1523089722	-0.3075814407
		O	-3.5760849533	-0.2881975908	0.1084055921
		O	-2.3823934090	1.4375325111	-0.6525168717
		C	-1.2808387245	-0.6508715132	-0.5324066693
		C	-0.0269960950	0.0536802227	-0.0559505687
		H	-1.4203299699	-1.6119270852	-0.0364700476
		H	0.8857981919	-0.6520537444	-0.3031737649
		H	0.1482161394	1.0022722936	-0.5638359335
		H	0.0134844676	0.1882614784	1.0270114452
		C	-3.5458283763	2.2464783543	-0.4944815711
		H	-3.2626109962	3.2512049713	-0.8036839769
		H	-4.3602398083	1.8681664066	-1.1166093072
		H	-3.8733250775	2.2425354293	0.5475790602
		H	-1.2110383935	-0.8442642610	-1.6087620489
		O	1.8754361846	-1.4223845504	-0.8907703732
		H	2.1856138106	-0.7654178946	-1.5303825241
7.0	Yes	C	0.0863812733	-0.1045998219	0.0490267609
		O	0.0405481869	0.9293787318	0.6548948639
		O	-1.0577530689	-0.6605273172	-0.3720245297
		C	1.3790605921	-0.8260440484	-0.2699142979
		C	2.5729354297	-0.1253677722	0.3290959139
		H	1.3036083525	-1.8590593560	0.0937117336
		H	2.6557834667	0.9618611937	-0.1818746785
		H	2.4681051366	0.0679833293	1.3964320101
		H	3.5191927992	-0.6139466032	0.0957021309
		C	-1.0438410613	-1.8797372572	-1.0974410736
		H	-2.0809908030	-2.0842253011	-1.3595725687
		H	-0.4546009076	-1.7966892713	-2.0152296148
		H	-0.6620066608	-2.7051069504	-0.4889368160
		H	1.4764829586	-0.8965142252	-1.3594973484
		O	2.3126315371	2.1221167517	-0.7231104373
		H	1.4977507685	2.2226289177	-0.2044850487
9.6	Yes	C	-2.2146765701	0.4708307747	-0.1894703761
		O	-2.8947629126	0.3127707882	0.7869363296
		O	-2.4256469011	1.5478417242	-0.9560179372
		C	-1.0885967761	-0.4786284774	-0.5421413679
		C	0.1498669933	-0.1187695783	0.2637852106
		H	-1.4246185172	-1.4780209263	-0.2576633767

		H	-0.1163062606	-0.3045634391	1.4370057549
		H	0.9903790464	-0.7860072215	0.0738905881
		H	0.4481526939	0.9292196207	0.1903587329
		C	-1.6167161796	1.7981723159	-2.0957066409
		H	-1.8926336245	2.7919719181	-2.4457967419
		H	-0.5517019431	1.7916242894	-1.8452034274
		H	-1.8141168044	1.0732687772	-2.8910285423
		H	-0.8714314940	-0.4856857578	-1.6133240092
		O	-0.7461833971	-0.6296986930	2.5332983109
		H	-1.6445133533	-0.3998791148	2.2371534927
10.4	Yes	C	-2.5018422080	-0.1381162098	0.0871818405
		O	-2.5777219869	0.6221233282	1.0062807973
		O	-3.6031212353	-0.7973505314	-0.3164625754
		C	-1.2125069219	-0.4032189533	-0.6656668395
		C	-0.0705907540	0.3902283533	-0.0773268825
		H	-0.9967190482	-1.4768137050	-0.6445688444
		H	0.8768448385	0.1731216338	-0.7524961030
		H	-0.2520180959	1.4649306542	-0.0936580398
		H	0.2042329916	0.0741407262	0.9296470254
		C	-3.5377381797	-1.7056983681	-1.4030022940
		H	-4.5501346582	-2.0833868082	-1.5411288044
		H	-3.2144949870	-1.2125854445	-2.3246640905
		H	-2.8722509710	-2.5469900327	-1.1868388762
		H	-1.3557645571	-0.1491317480	-1.7219621109
		O	1.7564416197	0.0484890621	-1.8048929509
		H	1.8819401532	0.9939000435	-1.9699812518
11.2	Yes	C	-2.4048102796	0.3183192180	-1.0436599935
		O	-2.4210465422	1.5057313332	-1.1695367900
		O	-3.5132242738	-0.3897723054	-1.3283440196
		C	-1.1750571408	-0.4546920622	-0.6065481742
		C	-0.0833464945	0.4740619468	-0.1330147086
		H	-1.4409086690	-1.1631948832	0.1843817810
		H	-0.4321744575	0.8753133581	0.9241997431
		H	0.8700084205	-0.0323571516	0.0183024926
		H	0.0202697341	1.3660122587	-0.7514720978
		C	-3.5338651319	-1.7954385336	-1.1499712844
		H	-4.4983690223	-2.1328544508	-1.5279271725
		H	-2.7391190086	-2.2905955694	-1.7164080233
		H	-3.4533351351	-2.0663738917	-0.0926234726
		H	-0.8377917990	-1.0586186996	-1.4600600166
		O	-0.8340404228	0.8138347089	2.2486063979
		H	0.0342302226	0.6319967239	2.6355413385
11.7	Yes	C	-1.1846331447	0.8391051441	0.2910230561
		O	-2.0049892020	0.6144059329	1.1363379732
		O	-1.3029648241	1.9391506143	-0.4607622754
		C	-0.0097528721	-0.0965764323	0.0545144621

		C	1.2894089219	0.4341335851	0.6555739624
		H	-0.2987192317	-1.0295880712	0.5372448709
		H	1.0445775510	1.2480336533	1.4964944083
		H	1.8726511590	-0.3349914039	1.1610092883
		H	1.9121895404	0.9896325177	-0.0460879453
		C	-0.1922254100	2.4348106076	-1.1916370431
		H	-0.5818756388	3.2162907001	-1.8428233100
		H	0.5424610644	2.8657849422	-0.5048460454
		H	0.2739096142	1.6609229562	-1.8094323614
		H	0.1119732008	-0.2941798913	-1.0154970221
		O	0.4757012522	2.2675147459	2.1919716776
		H	-0.3701859806	1.8441903993	2.4129833037
11.9	Yes	C	-0.8414406860	1.2276710363	0.5185734881
		O	-1.1903272094	1.2143930959	1.6628996903
		O	-1.1783428637	2.2625873826	-0.2619848566
		C	-0.0237315940	0.0812294125	-0.0575422103
		C	1.3174204388	0.0004650744	0.6478462216
		H	-0.5997460750	-0.8244830256	0.1609978100
		H	1.9444340747	0.9424659418	0.3315202313
		H	1.2187882470	0.0720053127	1.7326784807
		H	1.8983360425	-0.8763859197	0.3595580449
		C	-0.6645752914	2.3842096118	-1.5825393749
		H	-0.9689971821	3.3718726751	-1.9276948444
		H	0.4268999499	2.3190323449	-1.5906464376
		H	-1.0976312928	1.6299999299	-2.2475251378
		H	0.1115237629	0.1385033637	-1.1377061785
		O	2.5610663772	1.9265503044	-0.4740363525
		H	3.2373793014	1.3543504596	-0.8648405745
12.6	Yes	C	-2.4013620135	0.4323680410	-0.2979926295
		O	-3.2746791814	0.2945150443	0.5053457727
		O	-2.4324710999	1.4904550241	-1.1293441241
		C	-1.2105903986	-0.5086510622	-0.3682653896
		C	-0.1211593240	-0.0044621358	0.5646303339
		H	-1.5699361193	-1.4797892359	-0.0264201633
		H	0.7710874652	-0.7770385166	0.5244903859
		H	0.3261748831	0.9451066252	0.2605259492
		H	-0.4594562895	0.0533613495	1.6003800149
		C	-1.4510623780	1.6476292445	-2.1406145212
		H	-1.6424184041	2.6181636507	-2.5972712359
		H	-0.4363234535	1.6434520621	-1.7315017571
		H	-1.5402327024	0.8717386876	-2.9071804400
		H	-0.8260185372	-0.6232761646	-1.3832964354
		O	1.6112841082	-1.8713568999	0.5391147669
		H	1.3212224450	-2.2478347140	1.3827464725
12.8	Yes	C	-1.1337956041	0.9884939178	0.4486540737
		O	-1.7931682188	1.6919723772	-0.2594449289

		O	-1.3106700687	1.0498376605	1.7774116938
		C	-0.0959056946	0.0331060890	-0.1147862835
		C	1.3427802523	0.4163731539	0.2159320386
		H	-0.2968477799	-0.9929539281	0.2124093432
		H	1.6944856006	-0.1701102138	1.1733045555
		H	2.0343940024	0.1251259830	-0.5754047548
		H	1.4786915848	1.4736787388	0.4560389451
		C	-0.5328933590	0.2660328071	2.6709426620
		H	-1.0888524151	0.2348560909	3.6076523200
		H	-0.3830944546	-0.7547151750	2.3115624235
		H	0.4428773977	0.7256868368	2.8499236265
		H	-0.2505361259	0.0636759934	-1.1948455137
		O	2.1523932779	-1.1197112146	2.0941074068
		H	2.9502496049	-1.3970311168	1.6216883921
13.2	Yes	C	-2.2735413447	0.4582623573	-0.2306492974
		O	-2.8350152517	1.0751477929	-1.0852782718
		O	-2.4206329009	0.8248985209	1.0578988340
		C	-1.3217185886	-0.6850019817	-0.5191344487
		C	0.1276885024	-0.2211544064	-0.3546191567
		H	-1.5201328177	-1.5295020331	0.1484043196
		H	0.6846854334	-1.0607488466	0.2457428760
		H	0.6607001065	-0.1097155829	-1.2988347630
		H	0.2272635610	0.6894394553	0.2401935546
		C	-1.9636173480	-0.0228665824	2.1036587808
		H	-2.5718620245	-0.9312592518	2.1617095667
		H	-0.9122929697	-0.3044165850	1.9929453015
		H	-2.0891874593	0.5445754265	3.0254274616
		H	-1.5157638454	-1.0104287228	-1.5400787466
		O	1.0266445090	-1.9231810840	1.3050562454
		H	1.7748894381	-1.4152184765	1.6512357442
TS-m [OH]					
Relative energy	Mirror image	Cartesian Coordinates (Å)			
0.0	Yes	C	-2.2469797805	0.4512073382	0.5402919631
		O	-2.0525307451	0.2456121026	1.7085429811
		O	-1.2750164813	0.3719484051	-0.3822095604
		C	-3.5687914273	0.8213278545	-0.0735629862
		C	-4.6788127052	0.8931227891	0.9612620015
		H	-3.4316637528	1.7741458575	-0.5960465025
		H	-4.8034500698	-0.0691698192	1.4618572417
		H	-4.4442017899	1.6318801947	1.7302376353
		H	-5.6257511903	1.1664529830	0.4924935670
		C	0.0032987448	0.0541549880	0.1034524733
		H	0.3191223710	0.7274852820	0.9026058122
		H	0.6871527204	0.0300376524	-0.7428881627
		H	-3.7813272014	0.0840079089	-0.8548791831

		H	-0.0143924928	-1.0414383324	0.5808710650
		O	-0.3378349733	-2.0908634400	1.3632503309
		H	-0.9170372268	-1.5924677647	1.9620433235
1.3	Yes	C	-0.3443274252	-0.7921838746	-0.8541167821
		O	0.0196651195	-1.7660201626	-0.2504274905
		O	0.2411780181	-0.3899259894	-1.9935662481
		C	-1.4601784526	0.1239928914	-0.4292399989
		C	-2.2857929400	0.6849127072	-1.5826834862
		H	-2.0704390441	-0.4369485681	0.2806572205
		H	-1.6655905158	1.2780635016	-2.2564566712
		H	-2.7436466205	-0.1180113593	-2.1657964874
		H	-3.0853618121	1.3220195452	-1.2000994607
		C	1.3041335123	-1.1871019945	-2.4466318106
		H	1.6769057781	-0.7546844695	-3.3732638651
		H	1.0212496485	-2.2376797199	-2.5347021500
		H	-0.9895885516	0.9403938705	0.1316615667
		H	2.1945454620	-1.1493814587	-1.6488890949
		O	2.8807788767	-1.2518298833	-0.4952770534
		H	2.1811599468	-1.7117230361	-0.0036961880
1.3	Yes	C	-2.0498123033	0.5547525675	0.5591690112
		O	-1.7030973741	0.1593663330	1.6400864806
		O	-1.2160205678	0.6014295618	-0.4929259297
		C	-3.4330918066	1.0305185347	0.2065343422
		C	-3.4404057681	2.3093758247	-0.6280483968
		H	-3.9186657535	0.2178332841	-0.3459944993
		H	-2.9352985779	3.1230156970	-0.1018798819
		H	-2.9305339472	2.1563591683	-1.5803237228
		H	-4.4662012702	2.6221785306	-0.8314044863
		C	0.0882863871	0.1386550261	-0.2584452399
		H	0.6472155069	0.2247413733	-1.1883238766
		H	0.0983427892	-0.8658831005	0.1686166924
		H	-3.9720569822	1.1519161704	1.1470836612
		H	0.6193729610	0.8468071231	0.5453260975
		O	0.8735438477	1.5296311165	1.6785133331
		H	0.1715648588	1.1140057893	2.2045994149
3.5	Yes	C	-2.1578936578	0.4076715472	0.4024286822
		O	-2.1071542331	-0.5676783944	1.0919539801
		O	-1.0642561905	0.9675541952	-0.1649493376
		C	-3.4039834642	1.1755605512	0.0513714314
		C	-4.6389799107	0.5841633683	0.7096673460
		H	-3.2413132602	2.2189597917	0.3413153757
		H	-4.7781282875	-0.4548625167	0.4045676099
		H	-4.5385059926	0.5919080129	1.7969191220
		H	-5.5313593908	1.1509897042	0.4380186357
		C	0.1541994981	0.3081948734	0.0643529352
		H	0.2060092513	-0.1282973629	1.0635770857

		H	0.9612973379	1.0072343907	-0.1475968884
		H	-3.4864416038	1.1819698019	-1.0408879996
		H	0.2489808374	-0.5900363263	-0.6838648222
		O	0.1466229069	-1.3687052642	-1.8598449124
		H	-0.2187848405	-0.6731593724	-2.4262452440
4.8	Yes	C	0.0090210920	-0.0186616201	0.0105442764
		O	0.1859377337	-0.5210849594	1.0805715151
		O	0.9909864468	0.1013014197	-0.9153691764
		C	-1.2875248422	0.5522784924	-0.4985033565
		C	-1.1527839945	2.0192199755	-0.9086200167
		H	-1.6006803436	-0.0477728101	-1.3595070593
		H	-0.8213739240	2.6311818900	-0.0656573024
		H	-0.4299249261	2.1300267106	-1.7191373276
		H	-2.1134130647	2.4088327008	-1.2506709675
		C	2.2613906773	-0.3517312729	-0.5255706957
		H	2.8584752989	-0.4968396562	-1.4241684377
		H	2.2072175236	-1.2370531321	0.1110520184
		H	-2.0254526639	0.4218488665	0.2937756019
		H	2.7765923746	0.4791173360	0.1228546567
		O	3.1475416981	1.7562723282	0.6007013776
		H	2.7554689143	2.2688767310	-0.1214311064
4.9	Yes	C	-1.3893509916	-0.3641445919	1.2015065582
		O	-1.4356824867	-1.4893475309	1.6023076525
		O	-0.5544564224	0.0266236097	0.2087915365
		C	-2.2150015771	0.7899393213	1.7053304350
		C	-2.9278781400	1.5475730471	0.5862060270
		H	-2.9185128523	0.3812688874	2.4317483780
		H	-2.2089746508	1.9637643551	-0.1216769552
		H	-3.6038364825	0.8881325245	0.0359311754
		H	-3.5194470952	2.3669839771	0.9989189273
		C	0.2916310131	-0.9667259174	-0.3094691291
		H	0.6594867173	-0.6262921401	-1.2758222278
		H	-0.1937922105	-1.9438237003	-0.3461328940
		H	-1.5371563643	1.4646640667	2.2400478270
		H	1.2138348309	-1.0946724768	0.4038348745
		O	2.2699969331	-0.8007710243	1.2959786177
		H	2.1758747793	0.1628965927	1.2758661969
8.0	Yes	C	-0.7775689534	0.1969084229	1.9799718329
		O	-0.5406151740	0.2416405767	3.1477184673
		O	0.1074913324	-0.4457263595	1.1684651834
		C	-1.9979998816	0.8075295411	1.3338701703
		C	-2.8475087017	1.5444403726	2.3566282612
		H	-1.6651455146	1.4724261509	0.5287261503
		H	-3.1706743604	0.8686055948	3.1504388041
		H	-2.2730662789	2.3450096742	2.8264734018
		H	-3.7292123608	1.9786545291	1.8817484567

		C	-0.0864604434	-0.4763302984	-0.2131230762
		H	-1.0916349128	-0.7885658953	-0.5112703187
		H	0.6746686104	-1.1288350190	-0.6398000226
		H	-2.5712592415	0.0055895980	0.8530210597
		H	0.0728341144	0.5861010947	-0.6682147229
		O	0.3943557190	1.9869579249	-0.7936323216
		H	1.1472570470	1.9839630925	-0.1828873258
8.9	Yes	C	-0.8768942487	0.1480225287	2.1226695237
		O	-0.8221206287	0.0089670607	3.3052583153
		O	0.1248539392	-0.3753917297	1.3643013114
		C	-1.9892339046	0.8702862491	1.4004572914
		C	-2.9761855267	1.4774364886	2.3844421093
		H	-1.5451194968	1.6303223804	0.7477375074
		H	-3.4077680842	0.7059435895	3.0245812246
		H	-2.4741003049	2.1953469864	3.0356819779
		H	-3.7821420550	1.9891132587	1.8550208942
		C	0.1115048038	-0.2476576899	-0.0231282470
		H	-0.8283208961	-0.5709821786	-0.4807498399
		H	0.9559115017	-0.8156725998	-0.4134530565
		H	-2.4890140308	0.1525774252	0.7379077558
		H	0.2890793250	0.8628723274	-0.3246123362
		O	0.2962849672	2.2557731089	-0.7522204696
		H	-0.0632723604	2.1315347944	-1.6432639619
10.1	Yes	C	-1.2446705923	-1.3713207278	1.3203982477
		O	-1.2025239531	-2.2771201824	2.0931334010
		O	-0.1051364594	-1.0064139107	0.6752979527
		C	-2.4930880382	-0.5847354189	0.9956466130
		C	-3.6774697382	-1.0593155401	1.8209729338
		H	-2.2869904904	0.4790938124	1.1622468363
		H	-3.8717714820	-2.1177261591	1.6384282666
		H	-3.4716922254	-0.9472257744	2.8872014327
		H	-4.5742371894	-0.4881414814	1.5736173835
		C	-0.0967961324	0.0588031512	-0.2325184203
		H	-0.2273347806	1.0336186214	0.2454617476
		H	-0.7604207444	-0.0915905346	-1.0879028279
		H	-2.6907004143	-0.6848169806	-0.0783494746
		H	1.0195208572	0.0596109588	-0.6792731877
		O	2.2745381306	-0.3097634015	-0.8698598230
		H	2.2718392522	-1.0411614325	-0.2340400815
10.3	Yes	C	-0.8604723801	-0.4947055611	1.7130339695
		O	-0.9241779258	-0.8595901697	2.8466785839
		O	0.1773676042	0.3136266131	1.3579703531
		C	-1.9001421395	-0.8218759351	0.6676048997
		C	-2.9551746377	0.2898862166	0.6161965837
		H	-1.4435123631	-0.9922602378	-0.3095455162
		H	-3.4275865504	0.4059041985	1.5942005805

		H	-2.5210228001	1.2550789393	0.3403144148
		H	-3.7297300310	0.0478958479	-0.1138047150
		C	0.3785348029	0.6761205551	0.0250413798
		H	1.2057644888	1.3847794492	-0.0041413809
		H	-0.5125630363	1.0808901702	-0.4635397105
		H	-2.3626952545	-1.7559382050	0.9884976986
		H	0.6950465094	-0.2586452292	-0.5987998488
		O	0.9991475535	-1.6283071532	-0.9102979903
		H	1.5287391600	-1.8077814991	-0.1183963017
11.1	Yes	C	-1.4435101515	-1.3318735265	1.4792154292
		O	-1.6319279667	-1.9509522719	2.4813015334
		O	-0.1545332130	-1.0593026430	1.1356907543
		C	-2.5583498516	-0.8232961103	0.5956004738
		C	-2.8511356434	0.6566541270	0.8681409580
		H	-2.3350677291	-0.9905181170	-0.4613980837
		H	-3.1391914790	0.7928003657	1.9132599155
		H	-1.9849941366	1.2948035509	0.6775252002
		H	-3.6764526693	0.9997129489	0.2415056578
		C	0.1910254117	-0.2326138235	0.0656798448
		H	-0.5341930385	-0.2247722124	-0.7505799658
		H	1.1809466146	-0.5272713514	-0.2838965447
		H	-3.4271286130	-1.4318505242	0.8485695672
		H	0.2849234285	0.8687798424	0.4379866573
		O	0.3427645507	2.0211676158	1.2954294218
		H	0.4957874863	1.5273821295	2.1159231811
12.4	Yes	C	-1.2438093144	-1.4767269889	1.3204303815
		O	-1.2289432549	-2.4079727092	2.0637671607
		O	-0.0641316307	-1.0281711331	0.8139750566
		C	-2.5116802648	-0.7990923159	0.8555916229
		C	-3.0352424579	-1.4949605098	-0.4063857944
		H	-3.2329449369	-0.9083288468	1.6665035676
		H	-2.3199783401	-1.4331333123	-1.2314902617
		H	-3.2170150849	-2.5520132303	-0.2004855358
		H	-3.9715168971	-1.0404345030	-0.7353307241
		C	-0.0057772313	0.0812516001	-0.0379919387
		H	-0.0861765229	1.0314653528	0.4973017121
		H	-0.6785168339	0.0141377013	-0.8960586866
		H	-2.3555077182	0.2679786751	0.6776763920
		H	1.1057465872	0.0516733847	-0.4903517433
		O	2.3411050205	-0.3785899668	-0.7155649556
		H	2.3091458802	-1.1250381976	-0.0982372533

Table S4: Optimized geometries of the distinct conformers of the transition states (TSs) for MP H-abstraction by HO₂ and their energies (in kcal/mol) relative to the most stable conformation obtained using DFT-M08-HX/cc-pVTZ; the mirror image structure has the same relative energy as its corresponding conformer. The conformers with energies highlighted in bold are used in the semi-MS calculations.

TS- <i>a</i> [HO ₂]					
Relative energy	Mirror image	Cartesian Coordinates (Å)			
0.0	Yes	C	0.0004044841	0.0002752631	0.0005873289
		O	0.0178032791	-0.1823568112	-1.1971813677
		O	-1.0062816582	-0.3951826857	0.7782651269
		C	1.1146124905	0.6066504853	0.7594394309
		C	1.9093971606	1.6660419434	0.0603346287
		H	1.9307642183	-0.4935498298	0.6716292756
		H	0.9284806987	0.7166213638	1.8250353824
		H	2.2159402342	1.3210807025	-0.9302963108
		H	1.3076561184	2.5731682766	-0.0773290732
		H	2.7982333643	1.9318048387	0.6343893272
		C	-2.0570847359	-1.0837244420	0.1016395042
		H	-2.7953393196	-1.3305571243	0.8622853614
		H	-2.4956568324	-0.4461263153	-0.6690208204
		H	-1.6725125306	-1.9910912279	-0.3696776628
		O	2.4445964012	-1.4431791431	0.2136395147
		O	2.7424232799	-1.0841561407	-1.0800756125
		H	1.8882973474	-1.1476101534	-1.5355440338
0.6	Yes	C	-2.4911200434	1.4725387134	-0.2057660296
		O	-2.4704198905	1.2825155474	-1.3997934233
		O	-3.4843229595	1.0661700307	0.5849861733
		C	-1.3836002000	2.0914854051	0.5518834318
		C	-0.4841895922	3.0230030285	-0.2020236705
		H	-0.6619561941	0.9468864965	0.6578644115
		H	-1.6212398578	2.3288511254	1.5865298697
		H	-0.2869756819	2.6291617703	-1.2009175762
		H	-0.9557567410	4.0063336081	-0.3172902446
		H	0.4626761909	3.1689673047	0.3215709501
		C	-4.4908125518	0.2950760555	-0.0663197884
		H	-5.2255949441	0.0480328485	0.6977060843
		H	-4.9509004613	0.8684423920	-0.8740637720
		H	-4.0504858156	-0.6151980630	-0.4815072778
		O	-0.0948462162	-0.0676529757	0.4396742299

		O	-1.0597923333	-0.8966793991	-0.0849647654
		H	-1.0592527080	-0.6833808884	-1.0273096026
0.9	Yes	C	-1.1885335057	-0.4216898176	-0.4590445649
		O	-1.8759369002	-1.2239232283	0.1299678708
		O	-1.4719559481	0.0205448697	-1.6852066432
		C	0.0852525178	0.1106835306	0.0681575998
		C	0.8043684999	1.1980692490	-0.6701106710
		H	0.7910067521	-1.0418396345	-0.0867443135
		H	0.0816843141	0.1508103773	1.1556924558
		H	0.9270837296	0.9419630196	-1.7240232756
		H	0.2333611782	2.1339547313	-0.6271721290
		H	1.7863122489	1.3843550919	-0.2317899776
		C	-2.6164131378	-0.5787482394	-2.2879090532
		H	-2.7201873159	-0.1168033645	-3.2680390867
		H	-2.4645616190	-1.6564600191	-2.3862975047
		H	-3.5063148011	-0.4003845525	-1.6804172285
		O	1.1897967689	-2.1399802456	-0.2215706846
		O	0.2534312177	-2.7500261271	-1.0239257673
		H	-0.4330779996	-3.0272716408	-0.4023100265
0.9	Yes	C	-2.3887317043	1.4560571655	-0.1217714724
		O	-2.9233163423	0.4476803949	0.2848298655
		O	-2.8505640499	2.1433762413	-1.1660792395
		C	-1.1399820867	2.0144754325	0.4412555364
		C	-0.5816292815	3.2919381069	-0.1041205872
		H	-0.3312798864	0.9541965380	0.1335683131
		H	-1.0755359103	1.8427486065	1.5156617435
		H	-0.5074629218	3.2596476384	-1.1929661162
		H	-1.2364562173	4.1356659104	0.1478240790
		H	0.4051945931	3.4956908529	0.3145970620
		C	-4.0128004794	1.5926947269	-1.7848256518
		H	-4.2606976558	2.2590484642	-2.6088798673
		H	-3.8040544084	0.5855398322	-2.1520751894
		H	-4.8359078184	1.5416856787	-1.0688858671
		O	0.0176733891	-0.1555040838	0.0230140452
		O	-0.5093274427	-0.7729176129	1.1338342806
		H	-1.4504847768	-0.8574248924	0.9119420657
1.4	Yes	C	-1.1970185462	-0.3786376861	-0.8316133505
		O	-1.5185388082	-0.0237253159	-1.9332861646
		O	-1.9065883930	-1.2644008710	-0.1077688516
		C	0.0223471889	0.0645772546	-0.1174732183
		C	0.8329306308	1.1275219005	-0.7906266335
		H	0.7307780479	-1.0826177941	-0.1861391316
		H	-0.1024265018	0.1254264386	0.9628942796
		H	0.9634657387	0.8948129782	-1.8490218240
		H	0.3170873734	2.0937508171	-0.7318722331
		H	1.8107236865	1.2386865713	-0.3188070456

		C	-3.0659235712	-1.7647447451	-0.7706829574
		H	-3.5383952508	-2.4596645643	-0.0780986158
		H	-3.7479842879	-0.9479807950	-1.0173035618
		H	-2.7823824716	-2.2710878863	-1.6973235228
		O	1.2225698152	-2.1489307816	-0.2847389111
		O	0.3876670836	-2.8285698447	-1.1451875484
		H	-0.2499497346	-3.2434146762	-0.5527807097
1.4	Yes	C	-2.4525961126	1.5878151630	-0.2668965653
		O	-2.8833919418	2.0022141079	-1.3085017289
		O	-3.0621366192	0.6119818433	0.4386183892
		C	-1.1965355739	2.0363209907	0.3765265294
		C	-0.4709930725	3.1566225921	-0.2980822637
		H	-0.4793793869	0.8928575730	0.2926583565
		H	-1.2381408243	2.0314455545	1.4664932585
		H	-0.4120711579	2.9857556467	-1.3747506006
		H	-1.0116890365	4.1001418841	-0.1529616086
		H	0.5342708518	3.2784598366	0.1084598193
		C	-4.2655403038	0.1222278233	-0.1537990169
		H	-4.6546870177	-0.6346871143	0.5254144654
		H	-4.9860136171	0.9339119709	-0.2743836013
		H	-4.0577400362	-0.3104812662	-1.1349714524
		O	-0.1215257493	-0.2225897307	0.4054894670
		O	-0.6284725556	-0.6037481278	1.6287898940
		H	-1.5448388465	-0.8301857472	1.4255036583
1.9	Yes	C	-0.0435927689	-0.1200565082	0.1031493051
		O	-1.0898875986	-0.3307628335	0.6523041230
		O	0.2385757879	-0.5906885291	-1.1307096482
		C	1.0943059495	0.6307507795	0.6849946134
		C	1.8734312293	1.5590057454	-0.1995382883
		H	1.9523478339	-0.4063201942	0.8745282488
		H	0.8734236407	0.9676438941	1.6951903259
		H	2.2519723403	1.0358977861	-1.0805339224
		H	1.2393608918	2.3842922737	-0.5474367992
		H	2.7189050901	1.9879619724	0.3407320590
		C	-0.8255645773	-1.3253496211	-1.7362507030
		H	-0.4710707282	-1.6195438957	-2.7229680696
		H	-1.0714322654	-2.2039743851	-1.1355402422
		H	-1.7170192126	-0.7003430371	-1.8212221656
		O	2.6332314651	-1.3538870573	0.7388667769
		O	3.1228131634	-1.2451810939	-0.5451094601
		H	2.4125277589	-1.6125572960	-1.0856891535
2.2	Yes	C	-2.5164612914	1.5555742214	-0.2378320034
		O	-2.6641227951	1.7067884940	-1.4219663967
		O	-3.3702589440	0.8709114142	0.5325792719
		C	-1.3655386827	2.0769508801	0.5383179349
		C	-0.4630729814	3.0221499264	-0.1884817905

		H	-0.6211183591	0.9619190237	0.6892993997
		H	-1.5948185993	2.2857681071	1.5820861414
		H	-0.1655716763	2.5966127174	-1.1501697324
		H	-0.9819934789	3.9651732395	-0.4000158048
		H	0.4271229623	3.2526822696	0.4016632794
		C	-4.4701287615	0.2945956431	-0.1664918185
		H	-5.0612104266	-0.2340767704	0.5792725207
		H	-5.0663458558	1.0731535529	-0.6483475758
		H	-4.1124568159	-0.3961500755	-0.9337176093
		O	0.1639171826	0.0826028597	0.7383287370
		O	0.9863476544	0.2902530300	-0.3482194197
		H	1.7393848687	0.7606714668	0.0253278661
2.5	Yes	C	-2.5967141255	1.5079818432	-0.2868159730
		O	-2.7972896560	1.7716146790	-1.4428010793
		O	-3.4484306739	0.7980757152	0.4653759657
		C	-1.3816574791	1.8932246278	0.4730495555
		C	-0.4766534048	2.8991634284	-0.1647598589
		H	-0.6660482663	0.7593474888	0.4480013524
		H	-1.5497356476	1.9726685269	1.5466835819
		H	-0.4453725370	2.7453494247	-1.2445704127
		H	-0.8379189927	3.9177000140	0.0207956242
		H	0.5349313970	2.8223645749	0.2428273497
		C	-4.6165241293	0.3535364316	-0.2191079933
		H	-5.1998811499	-0.2086652085	0.5079967992
		H	-5.1876299959	1.2066010349	-0.5929844071
		H	-4.3434590590	-0.2807284429	-1.0657741552
		O	0.1286015343	-0.1231452163	0.4687577391
		O	1.2797043589	0.4584106440	0.9567167159
		H	1.2587298265	0.2450754343	1.8959041958
2.7	Yes	C	-2.5120938923	1.3289056778	-0.1448834434
		O	-3.5755874079	1.1264540512	0.3748554303
		O	-2.1986870850	0.8719014368	-1.3732144063
		C	-1.3866163920	2.0600298444	0.4825163600
		C	-0.4655402888	2.8707042024	-0.3834775496
		H	-0.6423917481	0.9948658631	0.8468230302
		H	-1.6761696406	2.4858683068	1.4406323638
		H	-0.1235153657	2.2896568073	-1.2416674949
		H	-0.9779488213	3.7620835383	-0.7656966151
		H	0.4040056403	3.2074887370	0.1843840216
		C	-3.2302684161	0.1038029757	-1.9898820345
		H	-2.8472487061	-0.1968437751	-2.9639252300
		H	-3.4662263377	-0.7703291487	-1.3770105304
		H	-4.1367377026	0.7023993919	-2.1031818155
		O	-0.0004087107	0.0076834353	0.9317122991
		O	-0.8587931756	-0.9904438095	0.5235058712
		H	-0.6937669497	-1.0508955346	-0.4245842565

3.2	Yes	C	-2.4911281038	1.2020602509	-0.1498583319
		O	-3.3759049490	0.7943458018	0.5555471475
		O	-2.4531929984	1.0001821552	-1.4731574586
		C	-1.3095791325	1.9550355180	0.3385039472
		C	-0.5471428318	2.8172683605	-0.6210284310
		H	-0.4561986299	0.9446927857	0.5965630448
		H	-1.4739145327	2.3392463631	1.3430973434
		H	-0.2184638397	2.2373313661	-1.4865717484
		H	-1.1769600121	3.6350598892	-0.9930523632
		H	0.3252785774	3.2625839564	-0.1369215596
		C	-3.5362526167	0.2298075209	-1.9871856522
		H	-3.3662111532	0.1433903163	-3.0589639241
		H	-3.5546267934	-0.7573796491	-1.5196614528
		H	-4.4875153871	0.7284223678	-1.7870716210
		O	0.3939966108	0.1303525349	0.7131420850
		O	1.2088011045	0.3113587414	-0.3840220386
		H	1.9261736879	0.8570927212	-0.0444279860
3.3	Yes	C	-2.7291862386	1.5480926169	-0.0703092970
		O	-3.6065119168	0.9242933141	0.4677349176
		O	-2.8258605301	2.0200212937	-1.3198549778
		C	-1.4185634280	1.8527566196	0.5554723271
		C	-0.6029797496	3.0126501735	0.0691567227
		H	-0.6746384140	0.8000929933	0.1970537908
		H	-1.4564837581	1.6918206904	1.6319803488
		H	-0.5816197199	3.0442761682	-1.0208387063
		H	-1.0222967103	3.9604355653	0.4281322931
		H	0.4213371668	2.9357983902	0.4428378997
		C	-4.0509617939	1.7096491232	-1.9783721892
		H	-3.9819061872	2.1492090734	-2.9719489467
		H	-4.1831935406	0.6271787447	-2.0446034113
		H	-4.8961155695	2.1307120397	-1.4288882741
		O	0.1783756489	0.0091256847	-0.0517659927
		O	1.2785726157	0.4638246502	0.6445374226
		H	1.2528021252	-0.0448261411	1.4622870725
6.9	Yes	C	-2.4909508808	1.6677337412	-0.1866324705
		O	-2.5511052911	1.5682987489	-1.3845029047
		O	-3.4985210770	1.2066161394	0.5655202400
		C	-1.3037732997	2.2576290631	0.4911062962
		C	-0.3769911726	3.0383010126	-0.3912883712
		H	-0.6514642880	1.0952000820	0.7239590322
		H	-1.4583048115	2.6443015673	1.4962148909
		H	-0.1887586968	2.4970765392	-1.3198349301
		H	-0.8296196409	3.9997726131	-0.6618231315
		H	0.5695354531	3.2415708045	0.1131506856
		C	-3.3271101705	1.0667886920	1.9683613743
		H	-4.1834672295	0.4921469629	2.3189203409

		H	-2.4095071496	0.5167647739	2.1998626191
		H	-3.3240992271	2.0398197249	2.4703400378
		O	-0.1873578709	0.0081931373	0.6864621306
		O	-1.2412225213	-0.7906406193	0.2992640166
		H	-1.2231551257	-0.7566629831	-0.6658558562
7.1	Yes	C	0.0096053648	0.3192024964	0.0130980176
		O	-0.0339007279	0.2658974556	-1.1910612439
		O	-0.9787817342	-0.2410448193	0.7249480560
		C	1.1739216680	0.9000097561	0.7258531761
		C	2.0885701356	1.7389873060	-0.1106478351
		H	1.8311621780	-0.2993157051	0.8198442449
		H	1.0344538907	1.1909969860	1.7635274853
		H	2.4481495521	1.1660785906	-0.9701339860
		H	1.5511579317	2.6064071560	-0.5120271936
		H	2.9408664137	2.0919196826	0.4709559161
		C	-0.8542325400	-0.3728012766	2.1322325414
		H	-1.7080534358	-0.9670566356	2.4552035539
		H	0.0686565860	-0.8984402923	2.3986750289
		H	-0.8895979805	0.6002709235	2.6324172543
		O	2.1605143151	-1.3910223732	0.5186623983
		O	2.4604044678	-1.2980223216	-0.8183963665
		H	1.6015549150	-1.3656009290	-1.2620650475
8.8	Yes	C	-1.3383109665	-0.0617255521	-0.7563152897
		O	-1.5745886689	0.2931911882	-1.8773273330
		O	-2.2922715506	-0.6678397335	-0.0351281944
		C	0.0052229809	0.1395126945	-0.1348351644
		C	0.9711914785	0.9328607311	-0.9607612076
		H	0.5000934747	-1.0999211718	-0.0589289351
		H	0.0027786877	0.3457456198	0.9366572305
		H	0.9909765414	0.5644872373	-1.9876615151
		H	0.6548827880	1.9818313785	-1.0047495049
		H	1.9769241848	0.8985591716	-0.5372742323
		C	-2.0284195507	-1.0962646810	1.2941305546
		H	-2.9033324381	-1.6676874901	1.6015895910
		H	-1.1447621230	-1.7371167076	1.3492000274
		H	-1.9117756214	-0.2409162947	1.9678645573
		O	1.0067399706	-2.1564429363	0.1586162217
		O	1.3112696159	-2.1184766683	1.5061557326
		H	2.2404531969	-1.8661177854	1.5196914616
9.3	Yes	C	-2.1259756951	2.3253930271	-1.6674488511
		O	-2.1670157824	1.8707010793	-2.7751545231
		O	-3.2646038880	2.7171814339	-1.0691915043
		C	-0.8467054896	2.4663196023	-0.9105429932
		C	0.3934255139	2.0734534575	-1.6509084380
		H	-0.9456519336	1.5387012542	0.0576996831
		H	-0.7724758127	3.3629912789	-0.2943110544

		H	0.2140510131	1.1737445777	-2.2405723401
		H	0.6921871330	2.8688100008	-2.3438295022
		H	1.2193282334	1.8986908051	-0.9568584103
		C	-3.2414491622	3.2207596103	0.2568785441
		H	-4.2836219181	3.3231896508	0.5572329340
		H	-2.7381881110	2.5335690348	0.9440589182
		H	-2.7641565843	4.2056333086	0.3002648333
		O	-0.8728927485	0.7742801794	0.9619700805
		O	0.4678231881	0.7465527574	1.2870776163
		H	0.5295210436	1.3419699419	2.0417200072
12.7	Yes	C	-2.2422149958	1.4912552650	-0.6995517192
		O	-2.6567610176	0.3603621448	-0.7020164402
		O	-2.7114126698	2.3455971548	-1.6229093242
		C	-1.1751662475	1.9254708373	0.2534053143
		C	-0.2057087684	3.0350755056	-0.0452393162
		H	-0.4226308466	0.7867719331	0.2214282642
		H	-1.4801971158	1.7972715958	1.2923148246
		H	0.0245118868	3.0863244677	-1.1122411095
		H	-0.5748433886	4.0167325566	0.2717610693
		H	0.7297704012	2.8576244822	0.4916695217
		C	-2.7520912143	3.7433033648	-1.3634275771
		H	-3.6554001260	4.1176969280	-1.8458270349
		H	-2.8127005958	3.9491248372	-0.2910474066
		H	-1.8814876479	4.2490661727	-1.7874480668
		O	0.0302217486	-0.2771979625	0.2343118844
		O	-0.8799214643	-1.0081309067	0.9607025267
		H	-1.6355229384	-1.0619263762	0.3541745894
TS-β [HO ₂]					
Relative energy	Mirror image	Cartesian Coordinates (Å)			
0.0	Yes	C	0.1642117163	-0.8004807309	2.3891402329
		O	1.3380681988	-1.0514254423	2.2849927946
		O	-0.5069485291	-0.9545566780	3.5264535064
		C	-0.7239454834	-0.2645682915	1.2926161332
		C	-0.0166137370	-0.1241429568	-0.0199486089
		H	-1.5947510384	-0.9247072443	1.2191044200
		H	0.3866748166	-1.4063580014	-0.3377023728
		H	-0.6309275730	0.1901637528	-0.8592606654
		H	0.9728513265	0.3292715047	0.0161100583
		C	0.2581488308	-1.4609506218	4.6208639923
		H	-0.4285774262	-1.5311527253	5.4621273562
		H	0.6664916570	-2.4433037315	4.3742546494
		H	1.0831796523	-0.7838864910	4.8523102653
		H	-1.1214802259	0.6980395371	1.6461626890
		O	0.8479891499	-2.4524678258	-0.3137316379
		O	2.2029923704	-2.2056910738	-0.1469215281

		H	2.2572542944	-1.9886039799	0.7952267153
0.4	Yes	C	-0.0004092578	-0.0009883617	-0.0027476967
		O	0.0882109454	-1.1517583364	0.3462411383
		O	-1.0215732626	0.4587976638	-0.7189755336
		C	1.0213704579	1.0743964152	0.2787678972
		C	1.7946913524	1.4117762055	-0.9688401599
		H	0.4952447371	1.9627606550	0.6528522160
		H	2.3737888222	0.1881992731	-1.2961741016
		H	1.1983569352	1.6364564251	-1.8508967073
		H	2.6566767531	2.0590767323	-0.8289983957
		C	-1.9952873880	-0.5208503209	-1.0858290418
		H	-2.7451061058	0.0043730508	-1.6741290089
		H	-1.5276954848	-1.3138826328	-1.6730709138
		H	-2.4440762831	-0.9604028160	-0.1926475704
		H	1.6900173066	0.7099888936	1.0613202117
		O	2.6617484589	-0.9134585720	-1.3721457280
		O	2.8830450836	-1.3057317928	-0.0595380014
		H	2.0040789299	-1.6028714814	0.2246293961
1.9	Yes	C	-0.0736808087	-0.7642881693	2.2418219012
		O	-0.3376588163	-1.8409483875	2.7111032222
		O	1.0393870236	-0.0933339621	2.5263442837
		C	-0.9156567956	-0.0323877879	1.2244064567
		C	-0.1935350068	0.0315715946	-0.0964209585
		H	-1.8682601712	-0.5559256216	1.1373923327
		H	0.1210563110	-1.2730684315	-0.4082546914
		H	-0.7939453385	0.3344844680	-0.9508596385
		H	0.8016297758	0.4713034815	-0.0655501630
		C	1.9708655484	-0.7848481918	3.3584529932
		H	2.7894552907	-0.0906328648	3.5386174979
		H	1.4983591753	-1.0795966385	4.2975166642
		H	2.3356292052	-1.6762449001	2.8409950686
		H	-1.1055427597	0.9833023912	1.5972620895
		O	0.3567262410	-2.3950191866	-0.5232403595
		O	1.2823716747	-2.6704047962	0.4751281632
		H	0.7277894505	-2.9673099972	1.2086981378
1.9	Yes	C	-0.5081210369	1.4472079212	2.6478281649
		O	0.2696216496	2.2207520454	3.1257780200
		O	-0.4660685585	0.1243043922	2.8920687224
		C	-1.6165604309	1.8261210095	1.6922369752
		C	-1.0188326296	2.3802559451	0.4274086238
		H	-2.2537858386	0.9644458711	1.4820450908
		H	-0.2824534269	1.3110782030	-0.0288358240
		H	-1.7131704319	2.5705087101	-0.3871293880
		H	-0.2561890951	3.1432518529	0.5708777037
		C	0.6032041333	-0.2856824236	3.7502815258
		H	0.5015939356	-1.3630042180	3.8686555614

		H	1.5636808323	-0.0346252147	3.2959641573
		H	0.5236745002	0.2174787254	4.7156597189
		H	-2.2271656728	2.5900053044	2.1913565978
		O	0.2565685105	0.2928828383	-0.1183042397
		O	-0.7466386868	-0.6443534627	0.0939132097
		H	-0.6866437535	-0.8036304994	1.0453153800
2.8	Yes	C	0.1854043457	-0.6098681896	2.3190454776
		O	1.3738927392	-0.4564426109	2.3350239212
		O	-0.5012426508	-1.1851579883	3.3086580101
		C	-0.7229200477	-0.1462131129	1.2025939117
		C	0.0210166812	-0.0241656958	-0.0907926986
		H	-1.5784061637	-0.8235565813	1.1337722242
		H	0.3876709727	-1.3060584933	-0.3649930769
		H	-0.5666966487	0.2694194683	-0.9571494395
		H	0.9979428070	0.4488250841	-0.0164445898
		C	0.3033183934	-1.6633664070	4.3849484788
		H	-0.3833270061	-2.1035880691	5.1060086704
		H	1.0105192610	-2.4111266316	4.0189226292
		H	0.8628588892	-0.8422275239	4.8387454921
		H	-1.1328134943	0.8295342355	1.5061278347
		O	0.6023628631	-2.4519501604	-0.4430440339
		O	0.0863092799	-2.9708867973	0.7387016294
		H	-0.7641112208	-3.3309035265	0.4678375594
3.1	Yes	C	-0.7740668816	1.0912308923	0.3372119255
		O	-0.0843767778	2.0715568343	0.2957159669
		O	-1.6952946187	0.8785718928	1.2806903876
		C	-0.7382342502	-0.0393279611	-0.6633203834
		C	0.4433223607	0.0642383840	-1.5754564996
		H	-0.7403542713	-0.9901114325	-0.1183319885
		H	1.4602227923	-0.3099508021	-0.7647679527
		H	0.4967833866	-0.6754663364	-2.3714475560
		H	0.7322116733	1.0729449060	-1.8622875101
		C	-1.7970618483	1.9113418612	2.2586843096
		H	-2.5734285162	1.5963068877	2.9536814934
		H	-0.8442098162	2.0373113066	2.7777271791
		H	-2.0656612652	2.8591207966	1.7860914898
		H	-1.6845114525	-0.0122930267	-1.2226062223
		O	2.1400281531	-0.7884938343	0.0603523687
		O	1.5257610909	-2.0059936301	0.3306094804
		H	2.0135912411	-2.6258067380	-0.2207324881
3.7	Yes	C	-2.4713695909	0.7301968463	1.4811505905
		O	-2.9846424037	0.2566399651	2.4527561915
		O	-2.5525964848	0.1557073358	0.2666574315
		C	-1.7236160003	2.0451153235	1.4774122815
		C	-0.8034095281	2.2835581759	0.3184947175
		H	-2.5003295432	2.8243561441	1.5164438841

		H	0.0418041944	1.2096462255	0.2949310961
		H	-1.2311682003	2.1590113891	-0.6749619105
		H	-0.1404962434	3.1398215587	0.4150204457
		C	-3.3280360296	-1.0462304299	0.2396862320
		H	-3.3374039590	-1.3796292008	-0.7975283793
		H	-2.8773786784	-1.8018662701	0.8867744416
		H	-4.3444181031	-0.8491963438	0.5859947458
		H	-1.2002397284	2.1051075183	2.4345873179
		O	0.5001343026	0.1522424531	0.2248381612
		O	0.1047377503	-0.2844497975	-1.0318147052
		H	-0.7932977540	-0.5964728933	-0.8710215419
4.0	Yes	C	-2.3184091399	3.2167798412	2.0495448078
		O	-2.1690227427	4.3736336124	1.7729118265
		O	-3.1925722608	2.7848936000	2.9642937424
		C	-1.5751112519	2.0578962151	1.4169742624
		C	-0.4719054469	2.5149222565	0.5123356392
		H	-1.2153148743	1.4081157622	2.2196863602
		H	-0.2040235969	1.4295790640	-0.2756779992
		H	-0.7583016086	3.2616107092	-0.2247838271
		H	0.4917077423	2.7119944921	0.9769652675
		C	-3.9570685219	3.8128159767	3.5923726362
		H	-4.6189220944	3.3116561456	4.2964830491
		H	-3.2990464922	4.5117282755	4.1137160466
		H	-4.5348780546	4.3660162645	2.8485283009
		H	-2.3176231400	1.4706471466	0.8606721588
		O	-0.0961618353	0.4620718437	-0.9066718618
		O	-1.2603656238	-0.2510788352	-0.6415052992
		H	-0.9757160582	-0.8951763700	0.0146648895
4.5	Yes	C	-2.4682434995	3.1937980528	2.1483670319
		O	-3.6300824657	3.3766475356	2.3747921657
		O	-1.5091873791	4.0655572976	2.4865813132
		C	-1.8943842574	1.9620768905	1.4768418605
		C	-0.9236359195	2.2856901825	0.3763856970
		H	-1.3785999819	1.3842616783	2.2553286858
		H	-0.3084924378	1.0941191522	0.1527427708
		H	-1.3498746700	2.5245426941	-0.5961751098
		H	-0.0880864082	2.9225153353	0.6604376411
		C	-1.9759224998	5.2370937748	3.1526773220
		H	-1.0951010608	5.8446287183	3.3531282813
		H	-2.6814243826	5.7793159905	2.5191377891
		H	-2.4787594875	4.9700282178	4.0849461442
		H	-2.7343995983	1.3673013757	1.1185278565
		O	0.1885189035	0.0419338098	0.1751394780
		O	0.4558674815	-0.1671688837	1.5227985061
		H	1.3773056627	0.0978711783	1.6077725664
4.5	Yes	C	-0.8540233889	1.5941153656	2.7278889993

		O	-1.1244331450	0.7791402510	3.5624402892
		O	0.3496201097	2.1551945752	2.5958997651
		C	-1.8223208915	2.1222217336	1.6883324602
		C	-1.1813016285	2.2698819797	0.3361479232
		H	-2.6760048359	1.4437016471	1.6700580324
		H	-0.4731644054	1.1220456479	0.1896720373
		H	-1.8551437539	2.2967002886	-0.5168799433
		H	-0.3505689414	2.9715578725	0.2826388102
		C	1.3708022224	1.5859603767	3.4121829576
		H	2.2791662174	2.1449172357	3.1950099001
		H	1.1069532493	1.6668504749	4.4689117181
		H	1.5022695397	0.5331803439	3.1506019334
		H	-2.1876902904	3.0971391973	2.0427288393
		O	0.1976637108	0.1661105156	0.2899231877
		O	1.4972621195	0.6554030007	0.3162347039
		H	1.7861631120	0.5566164943	-0.5966236135
4.5	Yes	C	-2.3662810438	3.2522244636	2.2068960858
		O	-2.3510399370	3.6558956464	3.3346549408
		O	-3.0721310302	3.8291742446	1.2281864656
		C	-1.6163047887	2.0308072162	1.7087851975
		C	-0.8145385876	2.3057521663	0.4684418534
		H	-0.9902347282	1.6873735224	2.5337143022
		H	-0.3765553034	1.0712659755	0.0780390407
		H	-1.3872231243	2.6231788035	-0.3999439958
		H	0.1156607368	2.8538534793	0.6076947722
		C	-3.8263271622	4.9720630305	1.6280236650
		H	-4.3341724616	5.3289243465	0.7338031813
		H	-4.5509477652	4.6989725751	2.3983855701
		H	-3.1643806221	5.7429610560	2.0287402682
		H	-2.3620172306	1.2535528623	1.5024741894
		O	-0.0994492820	-0.0310771809	-0.1547129034
		O	-0.9320599675	-0.7713960602	0.6762140929
		H	-0.3603327025	-0.9913101475	1.4188622743
4.8	Yes	C	-2.4352293370	3.1640256471	2.1866642704
		O	-3.5649180438	3.1793809759	2.5839836402
		O	-1.5812046909	4.1786895285	2.3599942225
		C	-1.7938578236	1.9924469417	1.4635792052
		C	-0.6835095142	2.3703805338	0.5286832093
		H	-1.4215952568	1.3226897238	2.2490072456
		H	-0.2978270898	1.1796358973	-0.0180735544
		H	-0.9758340666	2.9305282429	-0.3575973298
		H	0.2320154171	2.7329174261	0.9901713114
		C	-2.1173719285	5.2956941592	3.0675092936
		H	-1.3182197883	6.0328755488	3.1214502840
		H	-2.9812919353	5.7017566460	2.5367381653
		H	-2.4327256271	4.9953730611	4.0693452434

		H	-2.5963037676	1.4614170014	0.9471015982
		O	-0.0906718683	0.1087438408	-0.4127863513
		O	-1.3127386367	-0.5404250095	-0.2785971987
		H	-1.2010420425	-1.0507071646	0.5298877451
7.1	Yes	C	0.1036141184	-0.6834089655	2.3439848888
		O	1.2696334758	-0.9561161673	2.2680493195
		O	-0.5169809273	-0.8293782772	3.5194078963
		C	-0.7116355209	-0.1522571240	1.1816835130
		C	0.0830317579	-0.0860436552	-0.0867562142
		H	-1.6027051285	-0.7781345209	1.0559205151
		H	0.4233783023	-1.4061774558	-0.3393502606
		H	-0.4612169090	0.2336434884	-0.9712051190
		H	1.0919045436	0.3117828854	0.0037021747
		C	-1.9004175193	-0.5409037938	3.6519311451
		H	-2.1416856278	-0.7102644101	4.7002660574
		H	-2.1223312525	0.4999938547	3.3993905894
		H	-2.5087577413	-1.2084177912	3.0347804827
		H	-1.0920544306	0.8416179126	1.4638804768
		O	0.7842637673	-2.4818700468	-0.2481424205
		O	2.1449893231	-2.3520035141	-0.0166588241
		H	2.1724917687	-2.0976054192	0.9176957796
7.1	Yes	C	-0.5640809410	2.0254937483	2.7084384047
		O	0.6317397770	2.0808729510	2.6511541155
		O	-1.1487907814	1.6917071627	3.8661106027
		C	-1.4592424519	2.3469270780	1.5255490230
		C	-0.6781557550	2.3384789480	0.2489373303
		H	-2.2870909241	1.6345343287	1.4709497212
		H	-0.3702177235	1.0095962241	0.1316863664
		H	-1.2455264562	2.5333059669	-0.6575608643
		H	0.3042673225	2.8014849476	0.2932625400
		C	-2.5476827736	1.4543461278	3.9178034162
		H	-2.7801973214	1.2562121202	4.9633241437
		H	-3.1200016263	2.3254632602	3.5847407568
		H	-2.8136779971	0.5790603219	3.3164152165
		H	-1.9137228298	3.3330639601	1.7117555023
		O	-0.2562454223	-0.1460382978	0.2113583955
		O	-0.5546487314	-0.4394343913	1.5360174651
		H	0.2970376357	-0.3456534563	1.9807898645
8.2	Yes	C	-1.9674837178	-1.3061760450	0.6003288215
		O	-1.9723867517	-2.5073013132	0.6279862430
		O	-3.0419355487	-0.6717270450	0.1196521588
		C	-0.7733357303	-0.4817538960	1.0375160640
		C	0.1188406877	-0.1712596459	-0.1384315721
		H	-1.0876009879	0.4383065388	1.5452675888
		H	0.6411729687	-1.4363491608	-0.4576710074
		H	-0.3658624471	0.1050490330	-1.0735731579

		H	1.0107476713	0.4068503640	0.0892934533
		C	-3.1171853263	0.7469254027	0.1335475675
		H	-4.0181596771	1.0034816088	-0.4219804644
		H	-3.2089575401	1.1264163543	1.1557115852
		H	-2.2529071810	1.2058732631	-0.3544814468
		H	-0.2200647233	-1.0840435796	1.7640075566
		O	0.9065637098	-2.5291013760	-0.5720957212
		O	0.7665629855	-3.0611634338	0.6995240584
		H	-0.1849143917	-3.2535360693	0.7431462727
10.0	Yes	C	-2.6193020711	0.9840273602	0.9069845717
		O	-2.4895997206	-0.2083678980	0.8614861210
		O	-3.7280239595	1.5331994831	0.3981541571
		C	-1.5495038677	1.8994286575	1.4666510490
		C	-0.6148022797	2.3481328804	0.3682574106
		H	-1.9898384453	2.7604053866	1.9833560622
		H	0.0894254106	1.1881880128	0.0414156709
		H	-1.0579513631	2.5871396875	-0.5978975678
		H	0.1811929307	3.0226353136	0.6739122778
		C	-3.9477942425	2.9350237119	0.4693142549
		H	-4.8366159412	3.1289164082	-0.1295362647
		H	-4.1359705542	3.2530216683	1.4992014281
		H	-3.1076887210	3.4998115489	0.0554136202
		H	-0.9964354378	1.3163314966	2.2069647310
		O	0.5080214616	0.1450084186	-0.0971036722
		O	-0.3645693845	-0.4670467963	-0.9814939333
		H	-1.0554658149	-0.8098763400	-0.3957479162
10.5	Yes	C	-2.1752550106	3.0827046771	2.1270657474
		O	-1.8993496085	4.2045696281	1.8222118258
		O	-2.6626979407	2.8312663204	3.3545175591
		C	-1.9929547300	1.8952145518	1.1957537935
		C	-1.4884425422	2.3262537319	-0.1481506745
		H	-1.2810170082	1.1981620542	1.6583926580
		H	-1.0285812255	1.1609622682	-0.6794876462
		H	-2.2329994741	2.6564307706	-0.8689034267
		H	-0.5971825085	2.9498947629	-0.1292916737
		C	-2.9952462735	1.5073697974	3.7397556972
		H	-3.3203237077	1.5690338734	4.7776163061
		H	-3.8144693808	1.1060232430	3.1353858577
		H	-2.1326793287	0.8372424394	3.6767830772
		H	-2.9373113907	1.3490609875	1.1093972634
		O	-0.6002768524	0.1018051887	-0.9013781607
		O	0.1793256622	-0.1793452451	0.2159656983
		H	1.0632863199	0.0817289508	-0.0617879018
10.8	Yes	C	0.2485911413	0.0777801721	2.4019736329
		O	1.3754546913	0.4727288824	2.4764809536
		O	-0.3292566521	-0.4772706180	3.4729119716

		C	-0.5512754501	0.2356118499	1.1145868724
		C	0.2772317958	-0.2207471218	-0.0515180235
		H	-1.5083821797	-0.2879859927	1.1222879295
		H	0.2910430768	-1.5493145462	0.1612317878
		H	-0.1922979047	-0.1461887497	-1.0305773869
		H	1.3270149553	0.0623713741	-0.0146460689
		C	-1.5970558173	-1.1139135785	3.3760612961
		H	-1.7769950222	-1.5608658258	4.3532182280
		H	-2.3919823440	-0.3911017113	3.1667814610
		H	-1.5915760042	-1.8989135347	2.6148395624
		H	-0.7683667214	1.3097200359	1.0267500204
		O	0.0065625988	-2.6255690969	0.5634914312
		O	-1.3624887033	-2.7124112732	0.3274142805
		H	-1.4135384604	-3.1723852656	-0.5165439482
11.6	Yes	C	-1.3605206400	0.9193138427	1.7800582150
		O	-2.4855016168	1.3123275968	1.8647187164
		O	-0.3541188410	1.6728633531	2.2518314767
		C	-1.0034903380	-0.3919304211	1.1018320133
		C	-0.3837417386	-0.1638599027	-0.2587858635
		H	-0.3198959947	-0.9748055230	1.7357498242
		H	0.8585401300	-0.7084020406	-0.1975935891
		H	-0.8310531113	-0.7117441071	-1.0847504963
		H	-0.1373487535	0.8660674989	-0.5160082543
		C	0.9671945655	1.1489073610	2.3300242268
		H	1.5777240177	1.9473215218	2.7497594169
		H	1.0135475378	0.2788050491	2.9911545050
		H	1.3643106857	0.8740936603	1.3493642213
		H	-1.9317248413	-0.9577427725	1.0136804326
		O	1.9253252506	-1.1574009007	0.0000944704
		O	1.8092638472	-1.7908508558	1.2310531801
		H	1.6705388407	-2.7135373603	0.9923705043
12.4	Yes	C	-2.2215176751	3.1628113254	1.9453388330
		O	-1.8410273286	3.4337137683	3.0439637692
		O	-2.9693136753	4.0505070907	1.2659910752
		C	-1.8328599962	1.8616645901	1.2514080815
		C	-0.5382241351	2.0616542824	0.5079385779
		H	-1.6873543576	1.1287308636	2.0480250204
		H	-0.1398553311	0.7856345421	0.2327990428
		H	-0.5929725608	2.5048066369	-0.4854631146
		H	0.2829875601	2.4447577021	1.1121899352
		C	-3.4611976138	3.7444952299	-0.0278699162
		H	-3.9216739969	4.6595757665	-0.3990752861
		H	-2.6576114569	3.4514057037	-0.7102340762
		H	-4.2188338808	2.9556963025	0.0090218181
		H	-2.6129609009	1.4931141749	0.5831998585
		O	0.0860363268	-0.3472009150	0.1383086688

		O	-0.2853928505	-0.8673438974	1.3704296851
		H	0.5447288727	-0.8977641667	1.8573060274
12.4	Yes	C	-2.2222697051	3.3969736134	2.0103419978
		O	-3.2838273232	3.9034349781	1.8082837741
		O	-1.2458861457	4.1117258516	2.6011250177
		C	-1.8827398622	1.9859296888	1.5499501817
		C	-1.1791459653	2.0601804440	0.2170662466
		H	-1.2508597946	1.4679269522	2.2785630988
		H	-0.5491205476	0.8691902614	0.1394617141
		H	-1.8196589801	2.1121924026	-0.6603168261
		H	-0.3227688239	2.7340393455	0.1648229490
		C	-0.0499283543	3.4820132561	3.0366170795
		H	0.5973810294	4.2830458704	3.3923512763
		H	-0.2466558254	2.7900674860	3.8614648501
		H	0.4544180358	2.9408829776	2.2305825538
		H	-2.8246185548	1.4469369078	1.4574344410
		O	0.0823936243	-0.0893030975	0.3728370428
		O	0.8799135929	0.3122279888	1.4390393132
		H	1.7206655997	0.5169240732	1.0170812895
13.2	Yes	C	-1.3733157650	0.9444837456	1.6037110090
		O	-1.2662973995	1.5079803918	2.6506381414
		O	-2.1674074508	1.4727585500	0.6548353402
		C	-0.6344536444	-0.3526470118	1.2977747062
		C	0.5046144849	-0.1379426161	0.3355682295
		H	-0.2641414729	-0.7159050130	2.2553447661
		H	0.7264470856	-1.3790548772	-0.1417621280
		H	0.2685610860	0.3800939178	-0.5934801489
		H	1.4505147001	0.1726386344	0.7734155998
		C	-2.3213534868	0.9035819183	-0.6346145088
		H	-3.3531269242	1.0865831419	-0.9373678212
		H	-1.6536395526	1.4038995879	-1.3433890047
		H	-2.1305271708	-0.1719746125	-0.6544003421
		H	-1.3297510125	-1.1002019463	0.8989018102
		O	0.6005230785	-2.4600947138	-0.5807068574
		O	-0.6654794183	-2.4233498423	-1.1538422562
		H	-0.4787451373	-2.2794982548	-2.0872485348
14.9	Yes	C	-2.8456868061	1.0593855954	1.3978522021
		O	-2.8875713838	-0.0795559043	1.7490140504
		O	-3.9364912909	1.6163280718	0.8300208813
		C	-1.5921426953	1.9071393117	1.4895599426
		C	-0.8860110945	1.9710055810	0.1571041357
		H	-1.8241855243	2.9193260424	1.8438824056
		H	-0.1972989091	0.7999513018	0.0357643579
		H	-1.5130854536	1.9841016960	-0.7336560817
		H	-0.0302981019	2.6423811794	0.1048008523
		C	-3.9932500995	3.0116543091	0.5846800016

		H	-4.9390593864	3.1896519665	0.0738982024
		H	-3.9852770960	3.5798762210	1.5204775667
		H	-3.1744677478	3.3530601102	-0.0560736793
		H	-0.9462355152	1.4403881608	2.2366730039
		O	0.5513841116	-0.0801266713	-0.0242807648
		O	1.7029733391	0.5008299319	-0.5372814149
		H	1.6600556535	0.2791780966	-1.4729346615
15.5	Yes	C	-1.7925035005	-1.2877926878	1.0190500210
		O	-1.7807667070	-2.3936089650	1.4604766335
		O	-2.8156269803	-0.8941629678	0.2290358837
		C	-0.6715322938	-0.2907432770	1.2664384041
		C	0.2075724145	-0.1140708800	0.0558540238
		H	-1.0826145734	0.6802816584	1.5759740898
		H	0.6935499605	-1.3621316377	-0.2305560335
		H	-0.2946023607	0.0797743558	-0.8917593166
		H	1.1065645972	0.4790577311	0.2080550737
		C	-3.0429853960	0.4820410806	-0.0192272876
		H	-3.9033210387	0.5310953641	-0.6862273804
		H	-3.28444454564	1.0169488770	0.9055657516
		H	-2.1913365235	0.9666452643	-0.5059351480
		H	-0.0918554654	-0.6814707815	2.1040425151
		O	0.9179241126	-2.4440761372	-0.5515158660
		O	-0.2240894874	-2.8143265358	-1.2479208927
		H	0.0354336985	-2.6985994615	-2.1676834716
TS-m [HO ₂]					
Relative energy	Mirror image	Cartesian Coordinates (Å)			
0.0	Yes	C	0.0019942935	-0.0019044105	-0.0030481576
		C	1.4016933480	-0.0395737460	0.5411421069
		O	1.8930623913	-0.9548003340	1.1436462811
		O	2.0671953770	1.1018228016	0.2733436745
		C	3.3638487547	1.1985544693	0.7528286626
		H	0.0798349483	0.1949985714	-1.0776961357
		H	-0.4928237663	0.8775668667	0.4226821600
		H	3.7692774334	2.1790827042	0.5247470900
		H	4.1131355944	0.2515134111	0.1018904418
		H	3.4978904239	0.8219366944	1.7682849114
		O	4.5395279308	-0.7612200290	-0.2539956479
		O	4.6894346425	-1.4750799614	0.9236350507
		H	3.7835991367	-1.7573660800	1.1134958508
		C	-0.7587185430	-1.2841097265	0.2889464670
		H	-0.2491233557	-2.1441440419	-0.1498169396
		H	-1.7694332175	-1.2330600558	-0.1192963768
		H	-0.8260303919	-1.4582451337	1.3646525608
0.5	Yes	C	-3.1523061122	-0.5377902288	-0.7159886909
		C	-1.8465663713	-0.3493797678	0.0008391340

		O	-1.7002631369	0.1110689419	1.0977198203
		O	-0.8070774749	-0.7677375793	-0.7607720119
		C	0.4551742806	-0.5990245138	-0.2287159146
		H	-3.2008607961	-1.5778673506	-1.0544467170
		H	-3.0977739499	0.0693981167	-1.6266230653
		H	0.5146965247	-0.7676820049	0.8458359612
		H	0.7138689206	0.7339388533	-0.3448830662
		H	1.1902151341	-1.0976355845	-0.8535508949
		O	0.6995602603	1.8966663345	-0.4685190859
		O	-0.6339578266	2.1882498339	-0.7085961160
		H	-0.9971937733	2.2891004919	0.1795236227
		C	-4.3403125438	-0.1585421504	0.1515468825
		H	-4.3678069739	-0.7644682813	1.0596996388
		H	-5.2758396234	-0.3027704231	-0.3915155875
		H	-4.2758755380	0.8869113122	0.4598960907
1.3	Yes	C	-3.2117039155	-1.0677420230	-3.3118538170
		C	-1.8816802698	-1.0887988273	-2.6118009079
		O	-1.5330346983	-1.9025589158	-1.8004210093
		O	-1.0996845441	-0.0563260569	-2.9886846448
		C	0.1576172243	0.0206349846	-2.4113217832
		H	-3.8030462646	-0.2769686927	-2.8356411594
		H	-3.6987736121	-2.0180538516	-3.0894883885
		H	0.6753627057	-0.9367140033	-2.3316826725
		H	-0.0212679594	0.2493021341	-1.0695564305
		H	0.7080497119	0.8544208323	-2.8351655129
		O	-0.2970419048	0.1134888888	0.0428224884
		O	0.1934630395	-1.1470915424	0.3411624544
		H	-0.4755696228	-1.7286829189	-0.0468006587
		C	-3.1088047290	-0.8120057544	-4.8137691454
		H	-2.6462719014	0.1556680523	-5.0144051750
		H	-4.1019819138	-0.8190976997	-5.2662986373
		H	-2.5096933456	-1.5835416061	-5.3037450004
1.3	Yes	C	-2.8510581559	-1.2321325397	-3.0368160931
		C	-1.5107275543	-0.8264729034	-2.4929728422
		O	-0.8272411722	-1.4757964267	-1.7493086127
		O	-1.1441641304	0.3927351489	-2.9410712673
		C	0.0841633691	0.8733333891	-2.5166945824
		H	-3.0628609806	-2.2307694463	-2.6537531851
		H	-2.7663513892	-1.2919316869	-4.1269558832
		H	0.8825276167	0.1293270032	-2.5142902916
		H	-0.0035238464	1.0635642455	-1.1607873248
		H	0.2904665816	1.8283439019	-2.9892325610
		O	-0.1065244628	0.8681980740	-0.0272630713
		O	0.7884214579	-0.1641817655	0.2007006736
		H	0.3041550520	-0.9359966076	-0.1251341647
		C	-3.9462816826	-0.2347675026	-2.6528666513

		H	-4.0346219222	-0.1511979401	-1.5671364320
		H	-4.9095603171	-0.5618885503	-3.0479506150
		H	-3.7267434636	0.7560666064	-3.0547210958
1.4	Yes	C	-3.3482452500	-1.1895925349	-0.7901189339
		C	-1.9215362479	-1.2695489726	-0.3276508487
		O	-1.3655947679	-2.2384787427	0.1065579889
		O	-1.2982206837	-0.0708627462	-0.4537242243
		C	0.0025255146	-0.0009435428	0.0007723959
		H	-3.7934180086	-2.1702614786	-0.6177895260
		H	-3.3392585799	-1.0069924901	-1.8702593760
		H	0.5911637427	-0.8987717099	-0.1837203883
		H	-0.1020814056	0.0233234202	1.3591181079
		H	0.4428060583	0.9515256798	-0.2792076614
		O	-0.4114052549	-0.0438445349	2.4861966897
		O	-1.7228150219	-0.4907882620	2.4462964131
		H	-1.6257775225	-1.4504984210	2.4152603188
		C	-4.1191231617	-0.0772006206	-0.0762822172
		H	-4.0748648848	-0.2056165916	1.0079849335
		H	-5.1657580460	-0.0847067936	-0.3861219897
		H	-3.6939694804	0.8997933414	-0.3119346824
1.5	Yes	C	-1.9381134326	-0.7726255219	-0.2434243504
		C	-0.5782093720	-0.9747493158	0.3587667193
		O	-0.3144478386	-1.7233763580	1.2577130848
		O	0.3446084830	-0.1536175860	-0.1983440229
		C	1.6135759421	-0.1972642723	0.3440292287
		H	-2.4206455299	-1.7500484676	-0.3072121563
		H	-1.8358595839	-0.3543567068	-1.2462179683
		H	1.9405779759	-1.1942867190	0.6367163517
		H	1.5164906690	0.4491992917	1.5410871193
		H	2.2946446931	0.3956189571	-0.2591813437
		O	1.2087481544	0.9589441617	2.5461954407
		O	-0.1766253692	0.9478143389	2.5127863387
		H	-0.3969430243	0.0859986862	2.8877333557
		C	-2.7486684191	0.1660253024	0.6586680835
		H	-2.8563761106	-0.2690163451	1.6558820656
		H	-3.7458959532	0.3256579050	0.2451845712
		H	-2.2498412841	1.1324036494	0.7608764825
1.8	Yes	C	-4.2051792750	0.8605844116	0.0249811506
		C	-2.9070129073	0.6833856309	0.7601050876
		O	-2.4219831736	-0.3600890468	1.0958580650
		O	-2.2992602671	1.8730546760	0.9904324114
		C	-1.0580236836	1.8235485418	1.5918102950
		H	-4.7245152185	-0.0980044070	0.0661263397
		H	-3.9350223325	1.0456099029	-1.0218256439
		H	-0.7297988436	2.8265978375	1.8479029453
		H	-0.2107527776	1.3934338093	0.6137372669

		H	-0.9613595015	1.0534239660	2.3560444239
		O	0.3156597632	0.9561976153	-0.3339469924
		O	-0.7348432366	0.5531670226	-1.1429571164
		H	-0.9068426704	-0.3476465219	-0.8430306190
		C	-5.0664836349	2.0044920951	0.5543111070
		H	-5.3238218940	1.8499652150	1.6051339681
		H	-5.9961735434	2.0701448412	-0.0138261759
		H	-4.5436518035	2.9583024105	0.4693744867
2.1	Yes	C	-3.9874338509	-2.7609058276	-0.0317192583
		C	-2.7451607720	-2.6016739699	0.7959633825
		O	-2.6842865734	-2.2023526310	1.9177478503
		O	-1.6368680359	-2.9863086889	0.0933446017
		C	-0.4258741980	-2.7183009617	0.6923416878
		H	-3.9986785833	-3.7806052526	-0.4303457586
		H	-3.8708192655	-2.0991845732	-0.8972055756
		H	-0.4303856681	-2.8058572157	1.7778975288
		H	-0.2650470824	-1.3890907991	0.4949323953
		H	0.3772016277	-3.2149903309	0.1550339409
		O	-0.3942430477	-0.2539176303	0.1845284629
		O	-1.6248641538	-0.2257778410	-0.4531381018
		H	-1.3936044438	-0.3250916051	-1.3824246016
		C	-5.2414385553	-2.4351554029	0.7615543346
		H	-5.3411939468	-3.1023726375	1.6201957715
		H	-6.1311822462	-2.5361975505	0.1375368589
		H	-5.1961562045	-1.4142120821	1.1451204807
3.1	Yes	C	-3.3469597906	-1.1301795838	-0.7344883515
		C	-2.0255519270	-1.1793992575	-0.0196237826
		O	-1.6673075764	-2.0026456242	0.7644871533
		O	-1.2448612473	-0.1096462135	-0.3654827657
		C	0.0308534892	-0.0977531495	0.1543616475
		H	-3.8388396798	-0.1908172124	-0.4606929711
		H	-3.9468577211	-1.9567878496	-0.3523062806
		H	0.4818340488	0.8815157577	0.0192267290
		H	0.7230126203	-0.9414762013	-0.6479481210
		H	0.1193852354	-0.5587597550	1.1370153605
		O	1.0696052963	-1.6861356577	-1.4965339362
		O	-0.1180665781	-2.0332000625	-2.1202852130
		H	-0.1764802588	-1.4102610559	-2.8525548422
		C	-3.1886273416	-1.2102484036	-2.2538498174
		H	-2.5840610998	-0.3772134198	-2.6212419758
		H	-4.1652487552	-1.1630512045	-2.7394073380
		H	-2.7048357145	-2.1465551066	-2.5416344953
3.5	Yes	C	-2.9576453920	-1.3856643560	-3.1977719104
		C	-1.5134959541	-1.4133494358	-2.7836000244
		O	-0.9242003596	-2.3467205572	-2.3329340108
		O	-0.9169302742	-0.1955187949	-2.9674419011

		C	0.3493915448	-0.0636395226	-2.4423440617
		H	-3.4996146133	-0.9369911690	-2.3566473613
		H	-3.2821238381	-2.4247288423	-3.2716671974
		H	0.9502782666	-0.9710146664	-2.4820976483
		H	0.1241551682	0.0956235158	-1.1166249483
		H	0.8084200936	0.8559526244	-2.7946303226
		O	-0.3619748186	0.2106977859	-0.0440574522
		O	-1.7210856255	0.0830877683	-0.2845157754
		H	-2.0148313392	0.9951046432	-0.3784730080
		C	-3.2275117617	-0.6073663123	-4.4821992872
		H	-2.9291874336	0.4371029697	-4.3784102228
		H	-4.2910688241	-0.6387935464	-4.7264951025
		H	-2.6760838393	-1.0330981043	-5.3242437657
3.5	Yes	C	-3.2220451312	-0.9842645942	-0.4795323174
		C	-1.8350288102	-1.5217537156	-0.2591756628
		O	-1.5374320544	-2.6690202834	-0.1146974886
		O	-0.9184171730	-0.5155934858	-0.2497668040
		C	0.4005835518	-0.8794110107	-0.0532258631
		H	-3.2090646504	-0.4197080568	-1.4181447512
		H	-3.4173801241	-0.2446467358	0.3045016189
		H	0.6433023006	-1.8834465155	-0.3965689349
		H	0.5796631295	-0.9065266446	1.2810053772
		H	1.0574543842	-0.0674602227	-0.3539568696
		O	0.5412657800	-0.6906831863	2.4376751698
		O	0.1849441235	0.6483446568	2.4954676814
		H	-0.7722903488	0.6181587513	2.5902236552
		C	-4.2631287756	-2.0906445787	-0.4922768280
		H	-4.0497924590	-2.8121296920	-1.2835468382
		H	-5.2611897616	-1.6800076793	-0.6546981335
		H	-4.2593129812	-2.6359670065	0.4536679887
4.0	Yes	C	-4.5842221812	0.7041580344	0.1342626410
		C	-3.3099229242	0.6625804132	0.9299050034
		O	-3.0374330065	-0.1189899127	1.7896757788
		O	-2.4667488860	1.6621833453	0.5476283776
		C	-1.2255238679	1.6937982731	1.1483567639
		H	-4.3094008513	0.6008721496	-0.9210791026
		H	-5.0033853603	1.7110443461	0.2332679495
		H	-0.7788459395	2.6774341379	1.0285109001
		H	-0.4228543806	0.8639585890	0.4621354660
		H	-1.1953493137	1.2480347410	2.1426204242
		O	0.2663270624	0.0934032178	-0.1111322536
		O	0.9743249171	-0.5391930033	0.8987544129
		H	1.8188028745	-0.0777542398	0.8961691562
		C	-5.5624927127	-0.3711396182	0.5758319646
		H	-5.1201128187	-1.3631710145	0.4653045546
		H	-6.4773480956	-0.3284008905	-0.0176915191

		H	-5.8241235157	-0.2474915687	1.6287454822
5.4	Yes	C	-3.4246683925	-1.0977732245	-0.9071997194
		C	-2.0031059020	-1.3245762754	-0.4764024195
		O	-1.5225548643	-2.3539122199	-0.1115797960
		O	-1.2892635738	-0.1630930716	-0.5422732369
		C	0.0061346355	-0.1996899678	-0.0711642949
		H	-3.9106988242	-2.0734454120	-0.9381023292
		H	-3.4109971619	-0.6825193464	-1.9199080578
		H	0.4730570642	-1.1835759818	-0.1171933580
		H	-0.0501304474	0.0101819445	1.2538136416
		H	0.5711478986	0.6407510856	-0.4661228207
		O	-0.1337484770	0.1430308500	2.4258911454
		O	0.7452687240	-0.7990967302	2.9365035694
		H	1.5343328865	-0.2819399680	3.1265179190
		C	-4.1487288267	-0.1380214637	0.0403594200
		H	-4.1612270239	-0.5324116541	1.0591599258
		H	-5.1816230747	0.0053237194	-0.2819736395
		H	-3.6542166400	0.8350497161	0.0573590508
5.4	Yes	C	-4.7050999643	0.7231826727	0.4279545436
		C	-3.3762107214	0.6265878374	1.1248123413
		O	-3.0411737360	-0.2144218082	1.9021276571
		O	-2.5546549854	1.6500472733	0.7524687394
		C	-1.2736316080	1.6380508395	1.2628923897
		H	-5.3339476674	-0.0687832599	0.8364352505
		H	-4.5295256241	0.5002208620	-0.6303423459
		H	-0.8306279019	2.6273320933	1.1812875728
		H	-0.5249904873	0.8588843314	0.4642772771
		H	-1.1753515243	1.1220429756	2.2179580783
		O	0.1264249445	0.1362928656	-0.2061820946
		O	0.9146301739	-0.5471722719	0.7064593871
		H	1.7524118685	-0.0749157684	0.6691686889
		C	-5.3564949627	2.0984301159	0.5692253295
		H	-5.5304681133	2.3440520566	1.6198726087
		H	-6.3196206184	2.1150753865	0.0557348053
		H	-4.7231310721	2.8754627987	0.1378517711
5.9	Yes	C	-1.1698603971	-2.2818582722	0.8074361998
		C	-1.8341269583	-1.3307092374	-0.1553753779
		O	-2.9077699937	-1.4891627716	-0.6421065872
		O	-1.1563886385	-0.1762461876	-0.4712571886
		C	0.1194607330	0.0372604916	-0.0181115509
		H	-1.0889708838	-1.7773182032	1.7790969115
		H	-0.1472525329	-2.4730249817	0.4670731838
		H	0.4395592211	1.0438728617	-0.2774780552
		H	0.9000812866	-0.7811300650	-0.7612342328
		H	0.3168840612	-0.2573146233	1.0133938525
		O	1.3109122122	-1.6038036035	-1.5125216727

		O	0.1558035356	-2.2023320201	-1.9916992896
		H	-0.0663747094	-1.6851784092	-2.7735532237
		C	-1.9638126454	-3.5727317602	0.9258596222
		H	-2.9851735695	-3.3716718291	1.2533892755
		H	-1.4898698358	-4.2499363506	1.6386069688
		H	-2.0205208852	-4.0699430390	-0.0443568352
7.9	Yes	C	-1.1104921578	-1.7826882544	0.6031746148
		C	-1.4543635648	-1.6898595256	-0.8619149657
		O	-2.2957548931	-2.3313675678	-1.4065088674
		O	-0.7404057940	-0.7987399626	-1.6217863053
		C	0.2443400425	-0.0225540442	-1.0690063612
		H	-1.1328884357	-0.7777088933	1.0384496556
		H	-0.0718136615	-2.1254542681	0.6905862561
		H	0.9008090503	-0.5204784470	-0.3503975256
		H	-0.2887088720	0.9104378792	-0.2848844791
		H	0.7569743076	0.5297274823	-1.8537201686
		O	-0.7020374442	1.6299002641	0.5848839340
		O	0.0787242112	1.2851916080	1.6810361485
		H	0.7512249681	1.9734268601	1.6983567208
		C	-2.0556748648	-2.7304496693	1.3243203598
		H	-3.0864275781	-2.3807828186	1.2396101578
		H	-1.7951281908	-2.7976169340	2.3819706383
		H	-2.0133061225	-3.7288217087	0.8850561874
8.0	Yes	C	1.0475592942	-0.9868511573	1.3700107718
		C	0.4817832744	-0.3943524520	0.1047921122
		O	-0.5003268772	-0.7842065636	-0.4417304736
		O	1.1000664792	0.7173474298	-0.4215072622
		C	2.2657315618	1.2036927913	0.1110622074
		H	2.1388285470	-0.9456818910	1.3741515711
		H	0.7568834820	-2.0378711726	1.3575229423
		H	2.5369519006	2.1336296610	-0.3838526840
		H	3.2228688749	0.3196178268	-0.2509024735
		H	2.3205440506	1.2302192894	1.2002334148
		O	3.8186097610	-0.6256359944	-0.6499745344
		O	2.8096280312	-1.4864439851	-1.0542365789
		H	2.6778510869	-1.2680722745	-1.9833090603
		C	0.4473622303	-0.2881370078	2.5955268444
		H	0.6928661806	0.7776576181	2.6221009526
		H	0.8221241365	-0.7426738247	3.5143638099
		H	-0.6412220143	-0.3777872932	2.5864864404
8.3	Yes	C	-1.6690363457	-4.2219112003	1.3977207224
		C	-2.4130760840	-2.9151670603	1.3083059547
		O	-3.3771439948	-2.7263419724	0.6295317694
		O	-1.9574978642	-1.8761879836	2.0727644521
		C	-0.6096834398	-1.7929607672	2.3468234147
		H	-1.5196132232	-4.4665393957	2.4558415337

		H	-0.6726162692	-4.0617494132	0.9695581225
		H	-0.3957909218	-0.8745365563	2.8863565086
		H	-0.0993540494	-1.6345231751	1.0830065480
		H	-0.1429274061	-2.6958430556	2.7425983227
		O	-0.1730705674	-1.6203601618	-0.0880921514
		O	-1.0830817103	-0.6127405158	-0.3521546634
		H	-1.9380107513	-1.0646893589	-0.3725898347
		C	-2.4050847146	-5.3282187104	0.6588033246
		H	-3.4015283203	-5.4799713710	1.0781597772
		H	-1.8508290723	-6.2660040644	0.7240255542
		H	-2.5288192655	-5.0665072382	-0.3933023549
8.4	Yes	C	-1.0394324768	-2.4502828087	0.4340974915
		C	-1.8890823526	-1.3441314597	-0.1483195644
		O	-3.0319307770	-1.4681096336	-0.4574685672
		O	-1.2910334524	-0.1325010180	-0.3463010697
		C	0.0063552539	0.0849056101	0.0430285492
		H	-0.5229707350	-2.0826089513	1.3285233271
		H	-0.2456023481	-2.6784828796	-0.2884566281
		H	0.7168083104	-0.7044073441	-0.2093891510
		H	0.0035585086	0.1171993864	1.3954515351
		H	0.3120296055	1.0877793676	-0.2449651054
		O	-0.2264234982	0.0499988907	2.5563577376
		O	-1.6118543593	0.0874267512	2.6022330676
		H	-1.8576817373	-0.8257982333	2.7874852348
		C	-1.8763334239	-3.6862961223	0.7240707573
		H	-2.6713980152	-3.4580663501	1.4374518912
		H	-1.2553964717	-4.4838425078	1.1356961695
		H	-2.3577950308	-4.0465216976	-0.1863426752
8.9	Yes	C	-1.0869323499	-2.3611697609	0.4791854858
		C	-1.9585881838	-1.2750283545	-0.1044688029
		O	-3.1362205091	-1.3597520450	-0.2512562354
		O	-1.3303115812	-0.1403784791	-0.5362099001
		C	-0.0303137748	0.1327379405	-0.1892578553
		H	-0.4995811299	-1.9476582065	1.3076155418
		H	-0.3628374534	-2.6380256338	-0.2978615087
		H	0.2714244046	1.0796692478	-0.6306103676
		H	0.8598609771	-0.7338647488	-0.6879300333
		H	0.2079955700	0.0278764195	0.8733545802
		O	1.7634376705	-1.4878149008	-0.9001929593
		O	2.2263030803	-1.7952384414	0.3719521793
		H	1.8424119883	-2.6616893226	0.5446600560
		C	-1.9202208349	-3.5508752551	0.9270780208
		H	-2.6390132611	-3.2515230043	1.6920600554
		H	-1.2834660146	-4.3384829673	1.3344832937
		H	-2.4887345978	-3.9571474877	0.0888954498
9.9	Yes	C	-1.1147479812	-1.7294245089	0.2993801941

		C	-1.1001857731	-0.9446432552	-0.9846677566
		O	-2.0531898666	-0.7421405185	-1.6752940384
		O	0.1139119885	-0.4727419959	-1.4146963494
		C	0.9826367631	0.0481083028	-0.4780304757
		H	-2.1568195814	-1.9887399734	0.4866940453
		H	-0.7914827052	-1.0747302035	1.1151957877
		H	1.2119318629	-0.5924516252	0.3750554105
		H	0.2201522445	1.0697791133	0.0372937276
		H	1.8375643692	0.5002367624	-0.9729321028
		O	-0.7865557253	1.6456553359	0.1880824778
		O	-1.0922633000	2.1206829259	-1.0741367084
		H	-1.6359096070	1.4198454431	-1.4635261389
		C	-0.2389367954	-2.9819506980	0.2121325574
		H	-0.6003069020	-3.6505943707	-0.5723972048
		H	-0.2611257669	-3.5263796049	1.1576731086
		H	0.8014367759	-2.7362761293	-0.0150585338
10.1	Yes	C	-2.1701276433	-0.2457516295	1.7434539900
		C	-3.0072218921	0.7429941611	0.9708419901
		O	-4.1781782137	0.6314985972	0.7898352158
		O	-2.3955495808	1.8740741013	0.4920880827
		C	-1.0477487405	2.0751394849	0.6386739249
		H	-1.1567936343	-0.3257662168	1.3449480387
		H	-2.6601945985	-1.2118503082	1.6164756362
		H	-0.7864640955	3.0687607022	0.2807961487
		H	-0.3768231588	1.2336421861	-0.1417630867
		H	-0.6252144826	1.8091324141	1.6114378780
		O	0.2590165786	0.3531313997	-0.6556431568
		O	1.0473219153	-0.1197522962	0.3854416561
		H	1.8917395395	0.3187268036	0.2411660062
		C	-2.1560595252	0.1364065741	3.2291803121
		H	-1.7035911489	1.1183922323	3.3953702664
		H	-1.5879032234	-0.5971053125	3.8037646674
		H	-3.1753300959	0.1687841068	3.6204674307
10.4	Yes	C	-2.1391689648	-0.2537154518	1.8102697288
		C	-2.9452178451	0.7180755180	0.9786881401
		O	-4.1125166546	0.6016545795	0.7777117321
		O	-2.3108121367	1.8244795521	0.4875842077
		C	-0.9643554150	2.0136359332	0.6715205692
		H	-1.1044880367	-0.3276511891	1.4650667819
		H	-2.6202015634	-1.2256146658	1.6836242974
		H	-0.6668105887	2.9664987758	0.2401258572
		H	-0.3323979411	1.0944052223	-0.0897734676
		H	-0.5933855633	1.8311321164	1.6820595561
		O	0.0101564744	0.1764080766	-0.7585347991
		O	-1.1875861805	-0.2980299387	-1.2732710885
		H	-1.3434978522	-1.1042996397	-0.7690036703

		C	-2.1958546524	0.1570982219	3.2871481887
		H	-1.7534655190	1.1437031132	3.4516458656
		H	-1.6566006035	-0.5624197518	3.9056751316
		H	-3.2337309575	0.1955685280	3.6247079690
11.5	Yes	C	-0.5157243085	-2.1145892563	-1.8630552778
		C	-1.4950605353	-1.3469053856	-2.7148811744
		O	-2.3951732322	-1.8392018532	-3.3163888296
		O	-1.4054636631	0.0230839767	-2.6901692427
		C	-0.2264079751	0.6494123047	-2.3747186114
		H	0.4821998655	-1.6708990640	-1.8793673158
		H	-0.4580799420	-3.1203676832	-2.2805675884
		H	0.6457229366	0.2945044641	-2.9310996052
		H	0.1543213646	0.4644819131	-1.1051312146
		H	-0.3626344886	1.7291546889	-2.3921136223
		O	0.6842164958	0.4250214972	-0.0349778227
		O	1.5050076576	1.5435909700	-0.0503702861
		H	2.3729724641	1.1771077313	-0.2469880141
		C	-1.0482402268	-2.1585814200	-0.4236576804
		H	-1.1631691101	-1.1537168200	-0.0096052670
		H	-0.3580284953	-2.7077581837	0.2185021584
		H	-2.0204438073	-2.6555978799	-0.3990686058

Table S5. ZPE-corrected energies (in kcal/mol) of transition states (TSs) and products (Ps) relative to those of the reactants for MP H-abstraction by H, CH₃, and OH obtained at the MRACPF2/cc-pVDZ//DFT-M08-HX/cc-pVTZ level. The radical in square brackets denotes the radical formed from H-abstraction of MP.

	TS- α	TS- β	TS-m	P [MP- α]	P [MP- β]	P [MP-m]
MP + H	6.5	11.5	9.9	-9.5	-0.7	-3.5
MP + CH ₃	9.5	13.4	12.1	-12.5	-2.5	-5.4
MP + OH	1.0	2.6	0.3	-23.5	-10.9	-13.8