

Experimental and Theoretical Investigation of the Reaction of RO₂ Radicals with OH Radicals: Dependence of the HO₂ Yield on the Size of the RO₂ Moiety — Supporting information —

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Supporting information available:

- a) Tabulation of the relative energies of all conformers for each trioxide intermediate
- b) Quantum chemical characterization of the structures at the M06-2X/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//M06-2X level of theory

Relative energies of conformers
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Conformer Erel

CH3O3H.tt 0.00
CH3O3H.pm 2.36

Conformer Erel

C2H5O3H.ppt 0.00
C2H5O3H.ppp 0.03
C2H5O3H.ppm 0.67
C2H5O3H.pmt 2.26
C2H5O3H.pmp 2.53
C2H5O3H.pmm 2.90

Conformer Erel

C3H7O3H.pppp 0.00
C3H7O3H.pptp 0.17
C3H7O3H.pptm 0.17
C3H7O3H.pptt 0.24
C3H7O3H.pppt 0.18
C3H7O3H.pppm 0.40
C3H7O3H.ppmt 0.76
C3H7O3H.pppm 0.99
C3H7O3H.pmpp 2.36
C3H7O3H.pmtp 2.36
C3H7O3H.pmtm 2.34
C3H7O3H.pmtt 2.44
C3H7O3H.pmpm 2.60
C3H7O3H.pmpm 2.16
C3H7O3H.pmmm 2.59
C3H7O3H.pmmt 2.88
C3H7O3H.pmpm 3.33

Conformer Erel

C4H9O3H.ppppt 0.00
C4H9O3H.pptpt 0.16
C4H9O3H.pptmt 0.13
C4H9O3H.ppttt 0.23
C4H9O3H.ppptt 0.22
C4H9O3H.ppppp 0.34
C4H9O3H.pptmm 0.59
C4H9O3H.pptpp 0.44
C4H9O3H.ppttp 0.84
C4H9O3H.ppttm 0.85
C4H9O3H.ppmmt 0.41

C4H9O3H.ppptp 1.01
 C4H9O3H.ppptm 0.85
 C4H9O3H.ppmtt 0.83
 C4H9O3H.pppmt 0.87
 C4H9O3H.ppppm 1.29
 C4H9O3H.pptmp 1.36
 C4H9O3H.ppmmm 0.95
 C4H9O3H.pppmm 0.83
 C4H9O3H.pptpm 1.23
 C4H9O3H.ppmtp 1.49
 C4H9O3H.ppmtm 1.59
 C4H9O3H.pmppt 2.39
 C4H9O3H.pmtpt 2.28
 C4H9O3H.ppmmp 2.00
 C4H9O3H.pmtmt 2.32
 C4H9O3H.pmttt 2.46
 C4H9O3H.ppmpt 2.01
 C4H9O3H.pmppt 2.68
 C4H9O3H.ppmpp 2.78
 C4H9O3H.pmtpp 2.58
 C4H9O3H.pmpmp 2.67
 C4H9O3H.pmtmm 2.76
 C4H9O3H.pmttm 3.07
 C4H9O3H.pmmmt 2.55
 C4H9O3H.pmttp 3.06
 C4H9O3H.pmppt 3.39
 C4H9O3H.pmmtt 2.86
 C4H9O3H.pmpmt 3.28
 C4H9O3H.pppmp 2.64
 C4H9O3H.pmtmp 3.54
 C4H9O3H.pmmmm 2.98
 C4H9O3H.pmtpm 3.32
 C4H9O3H.pmpmp 3.64
 C4H9O3H.pmmtp 3.60
 C4H9O3H.pmpmm 3.33
 C4H9O3H.pmmtm 3.62
 C4H9O3H.pmpmt 3.43
 C4H9O3H.pmmmp 4.20
 C4H9O3H.pmpmp 5.05

Raw quantum chemical data
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OH

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -75.64558463
 E(CCSD/Aug-CC-pVTZ) (Hartree): -75.63969595
 T1 diagnostic: 0.010032
 E(MP2/Aug-CC-pVTZ) (Hartree): -75.62633139
 E(MP3/Aug-CC-pVTZ) (Hartree): -75.63789655
 E(PMP2/Aug-CC-pVTZ) (Hartree): -75.62832196
 E(PMP3/Aug-CC-pVTZ) (Hartree): -75.63903953
 E(PUHF/Aug-CC-pVTZ) (Hartree): -75.42491177
 E(UHF/Aug-CC-pVTZ) (Hartree): -75.42155904
 E(UM062X/Aug-CC-pVTZ) (Hartree): -75.73381017
 Point group : C*V
 Cartesian coordinates (Angs):
 O 0.000000 0.000000 0.107996
 H 0.000000 0.000000 -0.863971
 Rotational constants (GHz): 0.0000000 564.2418254 564.2418254
 Vibrational harmonic frequencies (cm-1):
 3769.1136 (SG)
 Zero-point correction (Hartree): 0.008587

HO2

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -150.72604292
 E(CCSD/Aug-CC-pVTZ) (Hartree): -150.70776038
 T1 diagnostic: 0.028799
 E(MP2/Aug-CC-pVTZ) (Hartree): -150.69255912
 E(MP3/Aug-CC-pVTZ) (Hartree): -150.69874647
 E(PMP2/Aug-CC-pVTZ) (Hartree): -150.69557501
 E(PMP3/Aug-CC-pVTZ) (Hartree): -150.70048285
 E(PUHF/Aug-CC-pVTZ) (Hartree): -150.24520737
 E(UHF/Aug-CC-pVTZ) (Hartree): -150.24028066
 E(UM062X/Aug-CC-pVTZ) (Hartree): -150.90809462

Point group : CS
 Electronic state : 2-A"
 Cartesian coordinates (Angs):
 O 0.055022 0.708334 0.000000
 O 0.055022 -0.599994 0.000000
 H -0.880350 -0.866714 0.000000
 Rotational constants (GHz): 629.2136600 34.6871500 32.8748300
 Vibrational harmonic frequencies (cm-1):
 1252.3111 (A') 1458.2887 (A') 3687.4120 (A')
 Zero-point correction (Hartree): 0.014576

CH3O2

 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -189.96049733
 E (CCSD/Aug-CC-pVTZ) (Hartree): -189.93414093
 T1 diagnostic: 0.027847
 E (MP2/Aug-CC-pVTZ) (Hartree): -189.90702947
 E (MP3/Aug-CC-pVTZ) (Hartree): -189.92274648
 E (PMP2/Aug-CC-pVTZ) (Hartree): -189.91015752
 E (PMP3/Aug-CC-pVTZ) (Hartree): -189.92458433
 E (PUHF/Aug-CC-pVTZ) (Hartree): -189.28655267
 E (UHF/Aug-CC-pVTZ) (Hartree): -189.28145234
 E (UM062X/Aug-CC-pVTZ) (Hartree): -190.20981111
 Point group : CS
 Electronic state : 2-A"
 Cartesian coordinates (Angs):
 C -0.987497 -0.480576 0.000000
 O 0.000000 0.561551 0.000000
 O 1.199179 0.067204 0.000000
 H -0.859473 -1.084492 0.894432
 H -0.859473 -1.084492 -0.894432
 H -1.949500 0.022404 0.000000
 Rotational constants (GHz): 53.5982700 11.5647700 10.1270600
 Vibrational harmonic frequencies (cm-1):
 131.9535 (A'') 512.7257 (A') 979.3410 (A')
 1146.3196 (A'') 1201.5411 (A') 1294.9751 (A')
 1458.0924 (A') 1485.2020 (A'') 1494.9065 (A')
 3087.8938 (A') 3178.9210 (A'') 3195.3532 (A')
 Zero-point correction (Hartree): 0.043666

CH3O

 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -114.88503865
 E (CCSD/Aug-CC-pVTZ) (Hartree): -114.87138374
 T1 diagnostic: 0.018331
 E (MP2/Aug-CC-pVTZ) (Hartree): -114.84389597
 E (MP3/Aug-CC-pVTZ) (Hartree): -114.86669911
 E (PMP2/Aug-CC-pVTZ) (Hartree): -114.84635299
 E (PMP3/Aug-CC-pVTZ) (Hartree): -114.86816675
 E (PUHF/Aug-CC-pVTZ) (Hartree): -114.47242060
 E (UHF/Aug-CC-pVTZ) (Hartree): -114.46839717
 E (UM062X/Aug-CC-pVTZ) (Hartree): -115.04237469
 Electronic state : 2-A
 Cartesian coordinates (Angs):
 C -0.576758 0.000000 -0.012094
 O 0.790789 0.000000 -0.007227
 H -0.997749 0.905435 -0.460177
 H -0.997749 -0.905435 -0.460177
 H -0.870264 -0.000000 1.050731
 Rotational constants (GHz): 158.2267200 28.0055000 27.8344500
 Vibrational harmonic frequencies (cm-1):
 405.1819 969.5691 1136.5838
 1385.0820 1386.8381 1519.1092
 2963.4431 3036.9864 3077.7963
 Zero-point correction (Hartree): 0.036179

C2H5O

 E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -154.13187417
 E (CCSD/Aug-CC-pVTZ) (Hartree): -154.11033298
 T1 diagnostic: 0.017322
 E (MP2/Aug-CC-pVTZ) (Hartree): -154.07229828
 E (MP3/Aug-CC-pVTZ) (Hartree): -154.10523548
 E (PMP2/Aug-CC-pVTZ) (Hartree): -154.07476833
 E (PMP3/Aug-CC-pVTZ) (Hartree): -154.10673557
 E (PUHF/Aug-CC-pVTZ) (Hartree): -153.52490772
 E (UHF/Aug-CC-pVTZ) (Hartree): -153.52089413

E(UM062X/Aug-CC-pVTZ) (Hartree): -154.35398426
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.171635	0.491111	0.006000
O	-1.260658	-0.364218	0.009418
C	1.186020	-0.202198	0.000693
H	-0.307985	1.066426	-0.934958
H	-0.261763	1.241225	0.811319
H	1.254278	-0.887292	-0.841621
H	1.322209	-0.770056	0.920348
H	1.992221	0.529968	-0.070585

 Rotational constants (GHz): 39.1677500 9.5354200 8.4700700
 Vibrational harmonic frequencies (cm-1):

239.1941	426.2228	712.2619
887.2365	981.3682	1052.0722
1089.0453	1252.0193	1371.9752
1394.5200	1404.8340	1488.7237
1501.5508	2893.4080	2962.8592
3064.9383	3135.1074	3155.6518

 Zero-point correction (Hartree): 0.066096

C2H500.p

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -229.20856895
 E(CCSD/Aug-CC-pVTZ) (Hartree): -229.17423877
 T1 diagnostic: 0.024946
 E(MP2/Aug-CC-pVTZ) (Hartree): -229.13727832
 E(MP3/Aug-CC-pVTZ) (Hartree): -229.16260599
 E(PMP2/Aug-CC-pVTZ) (Hartree): -229.14044224
 E(PMP3/Aug-CC-pVTZ) (Hartree): -229.16446429
 E(PUHF/Aug-CC-pVTZ) (Hartree): -228.33958830
 E(UHF/Aug-CC-pVTZ) (Hartree): -228.33443585
 E(UM062X/Aug-CC-pVTZ) (Hartree): -229.52284244
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.488389	0.643456	0.251193
O	-0.793531	0.421890	-0.381444
O	-1.430880	-0.560576	0.176537
C	1.447322	-0.472329	-0.089708
H	0.812449	1.605503	-0.140554
H	0.306111	0.720759	1.321609
H	1.594246	-0.536333	-1.166543
H	1.057482	-1.421095	0.272971
H	2.410733	-0.286106	0.382869

 Rotational constants (GHz): 18.0133400 5.7729200 4.9736400
 Vibrational harmonic frequencies (cm-1):

127.3461	237.6700	369.6039
546.5278	811.4455	881.9443
1029.4530	1110.8986	1192.8243
1266.3469	1328.1061	1389.2654
1414.0463	1488.0646	1494.8671
1509.9564	3077.4140	3098.5932
3146.6509	3154.2374	3169.2381

 Zero-point correction (Hartree): 0.072547

C2H500.t

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -229.20816113
 E(CCSD/Aug-CC-pVTZ) (Hartree): -229.17402829
 T1 diagnostic: 0.024867
 E(MP2/Aug-CC-pVTZ) (Hartree): -229.13703501
 E(MP3/Aug-CC-pVTZ) (Hartree): -229.16233690
 E(PMP2/Aug-CC-pVTZ) (Hartree): -229.14018069
 E(PMP3/Aug-CC-pVTZ) (Hartree): -229.16418590
 E(PUHF/Aug-CC-pVTZ) (Hartree): -228.34019928
 E(UHF/Aug-CC-pVTZ) (Hartree): -228.33507811
 E(UM062X/Aug-CC-pVTZ) (Hartree): -229.52240392
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.405828	0.534861	0.000178
O	0.630354	-0.474678	0.000376
O	1.812895	0.056782	-0.000316
C	-1.732417	-0.181786	-0.000237
H	-0.256014	1.146371	0.888593
H	-0.255427	1.146568	-0.887991
H	-1.831895	-0.808800	0.883874
H	-1.832591	-0.807049	-0.885478

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      H      -2.540594      0.547622      0.000874
Rotational constants (GHz): 33.9431800      4.4815100      4.1655800
Vibrational harmonic frequencies (cm-1):
      82.4796      231.3158      315.3122
      522.5750      802.9777      880.1082
      1057.3535      1154.3016      1161.0796
      1288.0996      1295.1038      1387.0561
      1424.6134      1490.4877      1501.5016
      1514.1144      3079.3324      3091.7924
      3138.4314      3156.4018      3162.9362
Zero-point correction (Hartree): 0.072303

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C2H5O3H.pmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -305.30578193
Electronic state : 1-A
Cartesian coordinates (Angs):
      C      1.198815      -0.563912      0.065268
      O      -0.090661      -0.946679      -0.395146
      O      -1.046332      -0.394161      0.478421
      O      -1.674585      0.654879      -0.202499
      H      -1.096035      1.409764      -0.026684
      C      1.440069      0.931474      0.016368
      H      1.353102      -0.955725      1.072662
      H      1.865119      -1.092381      -0.616513
      H      0.841372      1.448715      0.767566
      H      1.210888      1.326999      -0.972823
      H      2.484872      1.144947      0.239760
Rotational constants (GHz): 8.8498100      3.9153800      3.0415400
Vibrational harmonic frequencies (cm-1):
      133.7490      143.6388      291.5804
      338.0438      374.6305      502.3580
      580.2793      804.4201      890.0437
      936.9664      1009.2588      1088.8382
      1121.7813      1201.2065      1323.9898
      1386.7731      1413.4497      1424.8036
      1490.8338      1497.4867      1522.3023
      3060.7054      3069.6237      3116.9432
      3136.9141      3146.8100      3785.9857
Zero-point correction (Hartree): 0.088378

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C2H5O3H.pmp

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E(RM062X/Aug-CC-pVTZ) (Hartree): -305.30610791
Electronic state : 1-A
Cartesian coordinates (Angs):
      C      0.934488      0.417201      0.536110
      O      -0.094099      0.875049      -0.333950
      O      -0.940077      -0.195749      -0.645853
      O      -1.897830      -0.289357      0.380429
      H      -1.554926      -1.008153      0.927530
      C      1.862251      -0.580244      -0.123532
      H      1.456466      1.335615      0.803499
      H      0.482672      0.018884      1.449031
      H      2.312681      -0.144852      -1.013894
      H      1.322486      -1.479653      -0.413645
      H      2.656236      -0.863124      0.567001
Rotational constants (GHz): 11.0937300      3.1198500      2.9976300
Vibrational harmonic frequencies (cm-1):
      67.5508      158.7273      237.7264
      331.5178      362.3158      529.9180
      578.0335      803.7944      892.6930
      927.7081      998.6759      1089.2929
      1119.9108      1200.8628      1318.8402
      1384.8408      1406.0245      1418.7596
      1488.9111      1497.2216      1512.5945
      3053.7746      3074.4810      3119.6624
      3147.5831      3157.3699      3797.6219
Zero-point correction (Hartree): 0.088111

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C2H5O3H.pmt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -305.30660374
Electronic state : 1-A
Cartesian coordinates (Angs):
      C      0.859853      0.301430      0.401481
      O      0.005329      -0.615665      -0.270828

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O	-1.267015	-0.553722	0.303641	
O	-1.963117	0.501412	-0.314906	
H	-1.872500	1.219165	0.325577	
C	2.236949	0.116149	-0.193920	
H	0.500215	1.320685	0.235922	
H	0.847005	0.081311	1.470729	
H	2.220043	0.319903	-1.262906	
H	2.584678	-0.903344	-0.038428	
H	2.938174	0.800602	0.280486	
Rotational constants (GHz):	15.9929200	2.6448000	2.5077700	
Vibrational harmonic frequencies (cm-1):				
86.7963	133.6554		238.8300	
290.1061	370.4174		445.3710	
610.1174	834.2891		897.3451	
946.4802	1024.0103		1081.0878	
1177.1208	1190.4229		1294.3453	
1393.4665	1408.7150		1424.9137	
1488.8375	1505.3697		1528.7255	
3047.2578	3078.1467		3094.2395	
3154.3049	3158.7589		3801.9038	
Zero-point correction (Hartree):	0.088177			

C2H5O3H.ppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -305.30931260

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.189247	-0.562752	0.081937
O	-0.097125	-0.935905	-0.409431
O	-1.070331	-0.419946	0.458004
O	-1.518628	0.795349	-0.085260
H	-2.172405	0.500388	-0.733703
C	1.460795	0.923814	0.005529
H	1.293533	-0.937916	1.101618
H	1.862865	-1.126168	-0.564370
H	0.795373	1.475000	0.665965
H	1.319678	1.288476	-1.010520
H	2.489378	1.117861	0.309713
Rotational constants (GHz):	8.6695100	4.0097700	3.0696000
Vibrational harmonic frequencies (cm-1):			
116.2486	150.4932		252.5520
335.7960	396.6610		474.0528
607.8774	803.8558		883.6974
936.3982	1001.5402		1089.1094
1122.3435	1201.8314		1326.0929
1392.6507	1419.4294		1424.5293
1485.4288	1490.5329		1505.7026
3071.1381	3075.0544		3119.4622
3146.7444	3164.8551		3793.2353
Zero-point correction (Hartree):	0.088364		

C2H5O3H.ppp

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -304.90758440

E(CCS(D)/Aug-CC-pVTZ) (Hartree): -304.85948028

T1 diagnostic: 0.014720

E(MP2/Aug-CC-pVTZ) (Hartree): -304.83237035

E(MP3/Aug-CC-pVTZ) (Hartree): -304.85088390

E(RHF/Aug-CC-pVTZ) (Hartree): -303.73276393

E(RM062X/Aug-CC-pVTZ) (Hartree): -305.31030367

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.929409	0.518900	0.444130
O	-0.104575	0.749273	-0.513268
O	-0.925881	-0.385273	-0.560316
O	-1.820581	-0.294625	0.519082
H	-2.484238	0.323442	0.183069
C	1.900369	-0.551571	-0.002011
H	1.411371	1.493080	0.524941
H	0.466879	0.281320	1.403271
H	2.350178	-0.284698	-0.957051
H	1.392549	-1.507877	-0.108248
H	2.692895	-0.664243	0.737325
Rotational constants (GHz):	11.3727500	3.1015700	2.9979500
Vibrational harmonic frequencies (cm-1):			
84.1342	163.5357		237.7358
330.9697	373.3210		527.1089

595.7088	805.5348	889.4626
929.2916	998.8796	1082.3385
1119.7929	1202.3194	1325.0965
1389.8761	1418.2141	1421.6785
1488.5162	1495.6437	1509.7820
3074.8151	3081.3749	3126.4505
3146.8571	3161.6170	3792.1148

Zero-point correction (Hartree): 0.088330

C2H5O3H.ppt

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -304.90769731
 E (CCSD/Aug-CC-pVTZ) (Hartree): -304.85974734
 T1 diagnostic: 0.014578
 E (MP2/Aug-CC-pVTZ) (Hartree): -304.83266113
 E (MP3/Aug-CC-pVTZ) (Hartree): -304.85115633
 E (RHF/Aug-CC-pVTZ) (Hartree): -303.73380029
 E (RM062X/Aug-CC-pVTZ) (Hartree): -305.31037720
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.877658	0.189276	0.474957
O	-0.008725	-0.560765	-0.354928
O	-1.270127	-0.573618	0.249652
O	-1.904927	0.634805	-0.084750
H	-2.239925	0.450227	-0.972904
C	2.224609	0.165912	-0.209594
H	0.492125	1.204947	0.572359
H	0.913949	-0.278885	1.459770
H	2.162966	0.626344	-1.194120
H	2.579933	-0.856688	-0.324299
H	2.947574	0.719551	0.387218

Rotational constants (GHz): 15.6332800 2.6643000 2.5384400
 Vibrational harmonic frequencies (cm-1):

89.3441	150.3292	244.6715
295.6330	385.8752	441.0677
622.2048	828.8551	890.4748
946.3856	1023.0696	1077.9776
1172.3411	1191.6934	1292.7229
1394.1783	1420.2735	1424.1966
1489.8341	1505.7868	1532.3610
3069.5547	3076.9719	3115.2340
3153.4615	3156.2920	3792.7472

Zero-point correction (Hartree): 0.088355

C3H7O.p

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -193.37473376
 E (CCSD/Aug-CC-pVTZ) (Hartree): -193.34544693
 T1 diagnostic: 0.015805
 E (MP2/Aug-CC-pVTZ) (Hartree): -193.29758693
 E (MP3/Aug-CC-pVTZ) (Hartree): -193.34010095
 E (PMP2/Aug-CC-pVTZ) (Hartree): -193.30004681
 E (PMP3/Aug-CC-pVTZ) (Hartree): -193.34159119
 E (PUHF/Aug-CC-pVTZ) (Hartree): -192.57327838
 E (UHF/Aug-CC-pVTZ) (Hartree): -192.56925926
 E (UM062X/Aug-CC-pVTZ) (Hartree): -193.66227415
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.838051	0.443789	0.274561
O	1.466071	-0.677661	-0.197701
C	-0.567733	0.661549	-0.264582
H	0.819168	0.320261	1.372963
H	1.492769	1.311893	0.107862
C	-1.500901	-0.481488	0.108423
H	-0.945590	1.610285	0.122434
H	-0.507024	0.761982	-1.349743
H	-1.613303	-0.552664	1.191573
H	-1.100286	-1.428923	-0.250318
H	-2.490804	-0.344652	-0.323574

Rotational constants (GHz): 15.3738000 5.2853800 4.4799900
 Vibrational harmonic frequencies (cm-1):

132.5894	223.7595	312.7553
320.4326	494.1173	787.8818
884.5308	974.4226	999.0751
1095.1543	1116.3580	1221.2137
1292.0876	1365.4595	1367.2292
1387.1506	1420.2135	1484.5668

1502.0355	1510.6926	2938.3103
2991.2682	3061.5667	3064.9963
3100.7854	3131.7274	3144.3558

Zero-point correction (Hartree): 0.094145

C3H7O.t

 E(UM062X/Aug-CC-pVTZ) (Hartree): -193.66180679
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.690825	-0.424043	-0.009155
O	1.936940	0.138989	0.004467
C	-0.471325	0.555520	-0.005684
H	0.630413	-1.123774	-0.858786
H	0.651753	-1.082455	0.877641
C	-1.810599	-0.169151	0.005184
H	-0.376183	1.203597	0.866472
H	-0.389565	1.193420	-0.886937
H	-1.909200	-0.796382	0.892540
H	-1.914328	-0.813699	-0.869028
H	-2.641809	0.533420	0.000292

Rotational constants (GHz): 27.9607800 3.9695000 3.7127500
 Vibrational harmonic frequencies (cm-1):

117.5360	230.2501	245.4509
283.0408	481.5270	766.9155
897.7931	958.0724	1051.4085
1081.3529	1136.7519	1236.5205
1300.8960	1317.6995	1372.4815
1410.7584	1416.3774	1493.7643
1506.3650	1510.0135	2939.5452
2969.0982	3058.3133	3072.5364
3105.4887	3127.7854	3142.0880

Zero-point correction (Hartree): 0.093928

C3H7OO.pm

 E(UM062X/Aug-CC-pVTZ) (Hartree): -268.82986740
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.211582	0.952039	0.342862
O	-1.227598	0.251441	-0.407731
O	-1.534441	-0.889061	0.132928
C	1.169102	0.594518	-0.170806
H	-0.436210	2.006726	0.192213
H	-0.346269	0.681479	1.389069
C	1.528019	-0.871105	0.033321
H	1.227536	0.858631	-1.228072
H	1.880459	1.235973	0.353930
H	0.848110	-1.522142	-0.513813
H	1.468810	-1.143275	1.087388
H	2.540648	-1.069147	-0.314552

Rotational constants (GHz): 8.5357500 3.8614900 2.9668500
 Vibrational harmonic frequencies (cm-1):

111.1114	118.0066	244.6359
313.4057	440.4671	542.0191
776.2429	866.4589	926.6041
952.7220	1072.0900	1112.6911
1180.7973	1253.4996	1295.4307
1327.4613	1381.5168	1395.3557
1424.9934	1480.1747	1484.2125
1502.0334	1508.4407	3065.0926
3069.6238	3090.0310	3104.4887
3139.2837	3147.7250	3153.6660

Zero-point correction (Hartree): 0.101334

C3H7OO.pp

 E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -268.45124062
 E(CCSD/Aug-CC-pVTZ) (Hartree): -268.40901295
 T1 diagnostic: 0.022925
 E(MP2/Aug-CC-pVTZ) (Hartree): -268.36227111
 E(MP3/Aug-CC-pVTZ) (Hartree): -268.39710912
 E(PMP2/Aug-CC-pVTZ) (Hartree): -268.36543336
 E(PMP3/Aug-CC-pVTZ) (Hartree): -268.39897240
 E(PUHF/Aug-CC-pVTZ) (Hartree): -267.38707731
 E(UHF/Aug-CC-pVTZ) (Hartree): -267.38192555
 E(UM062X/Aug-CC-pVTZ) (Hartree): -268.83041476

Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.203310	0.933156	-0.211062
O	-1.114771	-0.126135	-0.587959
O	-1.743079	-0.597209	0.444811
C	0.968328	0.385634	0.575491
H	0.107692	1.360264	-1.164044
H	-0.779012	1.662052	0.356867
C	1.794190	-0.616050	-0.220957
H	1.583787	1.234383	0.879338
H	0.581329	-0.071052	1.486912
H	2.196522	-0.158589	-1.125767
H	1.186752	-1.469984	-0.517888
H	2.630482	-0.986764	0.368930

 Rotational constants (GHz): 9.7324400 3.2616700 3.0265800
 Vibrational harmonic frequencies (cm-1):

71.5771	152.2681	231.8270
294.4338	437.4146	562.5842
764.8521	881.4876	907.4822
960.4490	1065.6393	1115.8845
1182.9964	1250.2610	1301.7359
1316.1686	1375.5991	1401.3287
1421.1778	1481.2740	1489.5308
1505.4589	1509.1713	3065.7689
3073.9482	3089.2330	3112.7980
3136.5870	3146.6888	3150.2844

 Zero-point correction (Hartree): 0.101278

C3H7OO.pt

 E(UM062X/Aug-CC-pVTZ) (Hartree): -268.83011445
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.110585	0.659594	0.176412
O	-1.445452	0.411421	-0.314048
O	-1.977207	-0.620370	0.266503
C	0.863246	-0.371055	-0.352138
H	0.125298	1.662511	-0.177869
H	-0.157993	0.652657	1.265223
C	2.272044	-0.097226	0.158858
H	0.523410	-1.356811	-0.034201
H	0.840815	-0.352289	-1.442629
H	2.306497	-0.132214	1.248150
H	2.621323	0.886907	-0.155733
H	2.973691	-0.837039	-0.221372

 Rotational constants (GHz): 15.4035700 2.5486100 2.3982200
 Vibrational harmonic frequencies (cm-1):

100.8901	120.1496	234.1295
267.6621	383.8411	576.1854
763.8565	894.4263	904.6489
989.4545	1063.9164	1136.1533
1195.9191	1254.4592	1300.6953
1326.0588	1339.5790	1411.1141
1417.1361	1489.7586	1499.7367
1505.5676	1514.9730	3063.4179
3075.8809	3088.1258	3112.2313
3131.6076	3145.0471	3150.4361

 Zero-point correction (Hartree): 0.101281

C3H7OO.tp

 E(UM062X/Aug-CC-pVTZ) (Hartree): -268.82974886
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.196185	0.721424	0.286684
O	0.994382	-0.298858	-0.357188
O	2.205082	-0.322800	0.105819
C	-1.212234	0.605219	-0.248007
H	0.250434	0.539529	1.360313
H	0.658213	1.680339	0.055769
C	-1.881440	-0.707839	0.139232
H	-1.780980	1.451332	0.140822
H	-1.185353	0.715783	-1.333337
H	-1.934818	-0.808717	1.223887
H	-1.323171	-1.557866	-0.249942
H	-2.895105	-0.759963	-0.254008

 Rotational constants (GHz): 13.0956700 2.7777100 2.5071200

Vibrational harmonic frequencies (cm-1):

72.4397	134.4918	208.3033
304.2428	390.2806	536.1508
759.1237	897.5859	922.7907
956.5697	1085.0259	1135.3581
1168.6924	1260.1303	1298.0351
1308.9244	1374.5145	1408.2116
1420.3262	1482.7807	1497.3289
1509.0653	1511.5320	3067.5349
3073.2927	3081.9989	3109.0091
3136.9900	3141.6559	3149.2933

Zero-point correction (Hartree): 0.101154

C3H7OO.tt

E(UM062X/Aug-CC-pVTZ) (Hartree): -268.82947179
Electronic state : 2-A
Cartesian coordinates (Angs):

C	0.128551	-0.368242	0.000037
O	1.314862	0.455213	0.000011
O	2.394749	-0.262899	-0.000027
C	-1.073845	0.545339	-0.000001
H	0.170174	-0.998512	-0.888667
H	0.170185	-0.998502	0.888749
C	-2.365921	-0.262775	-0.000017
H	-1.029347	1.191414	0.877559
H	-1.029288	1.191388	-0.877576
H	-2.428687	-0.901407	0.881489
H	-2.428446	-0.901819	-0.881247
H	-3.234195	0.392993	-0.000291

Rotational constants (GHz): 23.1774400 2.2101200 2.0965700
Vibrational harmonic frequencies (cm-1):

77.4209	114.9169	203.8570
238.0249	408.7921	509.4180
760.0017	891.8359	931.2131
1011.3746	1070.7906	1164.9455
1169.2760	1262.5631	1296.2245
1320.0233	1332.2739	1417.5936
1419.6696	1497.6562	1504.1095
1506.6395	1517.6432	3064.2503
3072.8282	3081.3203	3106.7964
3128.4169	3141.8032	3146.1418

Zero-point correction (Hartree): 0.101077

C3H7O3H.pmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61361114
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.480189	1.214815	0.069848
O	0.655259	0.785499	-0.673124
O	1.579792	0.224834	0.227594
O	1.567378	-1.162388	0.034880
H	0.879798	-1.462519	0.645373
C	-1.301704	0.078534	0.651935
H	-0.156333	1.910175	0.846485
H	-1.059238	1.766764	-0.673017
C	-1.793682	-0.902409	-0.404879
H	-0.718134	-0.428844	1.425904
H	-2.148400	0.525100	1.177527
H	-0.959439	-1.333239	-0.957081
H	-2.436265	-0.395257	-1.125416
H	-2.367966	-1.711370	0.043996

Rotational constants (GHz): 5.2335100 2.6729600 2.0987000
Vibrational harmonic frequencies (cm-1):

107.3872	111.7840	183.6635
228.0272	280.8961	345.3430
431.9735	512.6848	595.5477
773.9390	877.0135	898.8461
933.5302	991.1141	1016.1205
1097.9589	1126.0702	1191.4103
1282.8345	1310.9509	1377.3445
1401.4980	1412.0216	1425.8619
1484.3061	1500.6750	1504.7851
1517.4055	3047.5983	3065.0106
3067.0923	3088.6368	3116.9616
3134.0252	3146.3344	3785.4822

Zero-point correction (Hartree): 0.117034

C3H7O3H.pmpmp

Cartesian coordinates (Angs):

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.420000
O	1.357953	0.000000	1.835168
O	1.749388	1.338827	1.954842
H	2.083178	1.531689	1.064736
C	0.714189	1.237012	-0.548303
H	0.521186	-0.902721	-0.318685
H	-1.042372	0.000000	-0.318685
C	2.169386	1.283464	-0.078044
H	0.676172	1.171164	-1.635648
H	0.174557	2.107784	-0.175940
H	2.652988	0.379543	-0.448391
H	2.151374	1.316163	1.011316
H	2.613110	2.183712	-0.503206

C3H7O3H.pmmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61311617

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.474197	0.919171	0.019084
O	0.893082	0.973367	-0.361236
O	1.625523	0.159080	0.523085
O	1.993210	-0.993472	-0.180497
H	1.228067	-1.574257	-0.067001
C	-1.112261	-0.449467	-0.135591
H	-0.582992	1.283281	1.044185
H	-0.944583	1.639479	-0.652757
C	-2.616574	-0.375152	0.098420
H	-0.898223	-0.830792	-1.135852
H	-0.672772	-1.136665	0.592526
H	-3.090564	0.281670	-0.631355
H	-2.837053	0.015277	1.092491
H	-3.078213	-1.357107	0.015473

Rotational constants (GHz): 7.3799400 1.9404600 1.6586000

Vibrational harmonic frequencies (cm-1):

98.6067	129.1285	146.4464
234.7172	262.8568	331.2290
375.4727	529.7129	584.7477
777.3678	895.1166	898.6724
935.0773	1006.9165	1053.9894
1092.0959	1138.6828	1207.0659
1293.9146	1320.0682	1334.4459
1412.9746	1420.9494	1427.7009
1488.8498	1501.9338	1505.7472
1517.2216	3046.6011	3056.3364
3064.7296	3091.8922	3115.4167
3132.2401	3145.7758	3785.7114

Zero-point correction (Hartree): 0.117008

C3H7O3H.pmpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61217595

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.394982	-1.008196	0.364200
O	0.573703	-0.744532	-0.647536
O	1.134423	0.522524	-0.437831
O	2.268675	0.347363	0.372811
H	1.932748	0.542477	1.257679
C	-1.753078	-0.402290	0.067520
H	-0.453077	-2.096620	0.392325
H	-0.004455	-0.671247	1.329250
C	-1.760655	1.120179	0.022817
H	-2.106645	-0.806268	-0.882704
H	-2.442293	-0.757631	0.837599
H	-1.138743	1.491505	-0.789374
H	-1.377352	1.541506	0.953683
H	-2.772304	1.495271	-0.125229

Rotational constants (GHz): 6.5007800 2.2073100 1.8964100

Vibrational harmonic frequencies (cm-1):

51.1153	107.9006	136.2261
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266.3565	304.1715	330.1526
381.5768	540.4363	580.7859
782.3056	861.9266	909.1856
927.7887	984.1314	1024.2501
1104.9295	1123.4212	1180.0408
1295.4090	1312.7439	1381.3494
1396.5087	1412.0662	1423.9636
1479.1822	1484.2237	1501.5463
1511.5990	3047.6563	3058.8603
3063.6884	3098.7742	3116.3567
3131.8181	3150.3183	3797.4160

Zero-point correction (Hartree): 0.116779

C3H7O3H.pmpp

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61381637

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.312443	0.931815	-0.363127
O	-0.481705	-0.106889	-0.926523
O	-1.194515	-0.748602	0.092655
O	-2.346503	0.016339	0.353027
H	-2.097392	0.513786	1.143197
C	1.345410	0.432104	0.629448
H	0.790608	1.369548	-1.240805
H	-0.342565	1.690860	0.073932
C	2.269444	-0.618797	0.029424
H	1.917998	1.297854	0.968758
H	0.838215	0.028274	1.506837
H	2.791803	-0.223711	-0.843050
H	1.702760	-1.492161	-0.288914
H	3.016572	-0.941967	0.752299

Rotational constants (GHz): 7.6758300 1.9606400 1.9118000

Vibrational harmonic frequencies (cm-1):

32.6366	88.4596	181.4714
234.3317	275.3197	365.3377
412.9284	561.4845	584.2824
771.0065	878.4682	896.7111
931.9704	975.8246	1018.3473
1099.2149	1123.8626	1191.8674
1291.6235	1304.1590	1379.1905
1399.3638	1407.5797	1422.4931
1483.0855	1493.4650	1505.6198
1509.9233	3051.3501	3065.6928
3069.9666	3098.8030	3115.5417
3135.1066	3149.2930	3798.1047

Zero-point correction (Hartree): 0.116879

C3H7O3H.pmpt

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61330800

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.380876	0.406511	0.589278
O	-0.826085	0.981527	0.107266
O	-1.521173	0.023838	-0.641256
O	-2.303928	-0.725154	0.255797
H	-1.773265	-1.521371	0.389618
C	1.376555	0.083027	-0.506742
H	0.772560	1.170720	1.262481
H	0.149198	-0.475195	1.196526
C	2.668174	-0.475492	0.077422
H	0.930768	-0.634205	-1.196365
H	1.574536	0.992765	-1.074927
H	2.481947	-1.392770	0.637867
H	3.133109	0.239695	0.757238
H	3.387019	-0.705601	-0.706649

Rotational constants (GHz): 8.5930800 1.6915400 1.6158300

Vibrational harmonic frequencies (cm-1):

63.9301	81.7315	157.0779
234.6275	274.0345	328.6913
360.7832	567.2363	577.0442
756.7252	883.6684	900.5125
926.1206	992.7558	1054.4618
1085.8580	1140.6390	1201.8266
1286.5121	1324.2957	1329.6417
1403.3009	1414.7289	1419.6324

1492.1197	1499.8099	1505.6022
1516.5601	3038.2473	3059.8757
3077.2612	3100.4950	3113.8845
3133.6361	3142.5945	3802.2930

Zero-point correction (Hartree): 0.116752

C3H7O3H.pmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61386720

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.289109	0.589292	0.381059
O	-0.383310	-0.447078	-0.324229
O	-1.625279	-0.673897	0.274211
O	-2.533846	0.257470	-0.261665
H	-2.562114	0.942017	0.419715
C	1.681225	0.691159	-0.209922
H	-0.255361	1.528589	0.251139
H	0.326541	0.329761	1.442530
C	2.513175	-0.563705	0.022666
H	1.590644	0.896905	-1.277626
H	2.166374	1.558374	0.241006
H	2.045049	-1.430210	-0.440380
H	2.615085	-0.766648	1.089587
H	3.512208	-0.451226	-0.395322

Rotational constants (GHz): 10.8931100 1.6486000 1.5345900

Vibrational harmonic frequencies (cm-1):

56.2408	101.5842	148.5128
202.2590	294.0787	327.2868
401.3495	475.7164	608.6691
765.4363	913.2993	936.9516
939.4019	976.4442	1037.7251
1097.7063	1156.9642	1186.5053
1267.8418	1313.2165	1379.5117
1402.2830	1411.7414	1423.3315
1483.0492	1500.2788	1511.1886
1522.6079	3039.9187	3066.9897
3070.2964	3089.0785	3109.5434
3136.6958	3151.2291	3801.6880

Zero-point correction (Hartree): 0.116885

C3H7O3H.pmtt

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61384840

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.328843	-0.668910	0.490091
O	-0.420091	-0.249665	-0.644306
O	-1.782237	-0.386738	-0.363863
O	-2.204292	0.790295	0.281058
H	-2.193030	0.537207	1.213494
C	1.793217	-0.535225	0.123002
H	0.092195	-0.021226	1.340865
H	0.063554	-1.700175	0.730743
C	2.209113	0.909149	-0.127235
H	2.376625	-0.962633	0.940170
H	1.986210	-1.146746	-0.759742
H	2.029310	1.521116	0.757746
H	1.642579	1.338499	-0.951206
H	3.268482	0.972740	-0.370337

Rotational constants (GHz): 8.0577300 1.7975800 1.6635900

Vibrational harmonic frequencies (cm-1):

53.7533	103.3028	152.1128
204.1537	294.8247	330.8250
401.4026	460.4374	614.8831
766.7156	909.9790	934.8735
941.8596	980.1157	1037.0772
1097.6695	1161.0649	1183.2108
1269.9912	1313.3975	1376.1268
1402.3158	1415.5164	1423.9356
1483.6407	1500.8240	1511.2664
1521.7020	3032.7486	3066.9138
3070.2582	3094.3960	3109.0365
3136.3469	3152.5144	3803.0063

Zero-point correction (Hartree): 0.116898

C3H7O3H.pmtt

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61371318
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.354140      0.108810      0.267726
  O     -0.684662     -0.758209     -0.165201
  O     -1.884908     -0.361584      0.431498
  O     -2.440257      0.657535     -0.364287
  H     -2.182048      1.459688      0.108458
  C      1.647072     -0.420178     -0.316523
  H      0.161840      1.123494     -0.095871
  H      0.385928      0.116297      1.360344
  C      2.827670      0.454963      0.085260
  H      1.794886     -1.443603      0.029601
  H      1.551959     -0.458248     -1.402125
  H      2.938994      0.490068      1.169437
  H      2.697536      1.477224     -0.271439
  H      3.756224      0.071579     -0.333271
Rotational constants (GHz):  11.4422700  1.4766800  1.4027400
Vibrational harmonic frequencies (cm-1):
  80.0030      88.5614      150.4681
 204.4800     240.4020     354.1643
 389.6656     460.3306     600.8173
 768.3987     912.7853     929.7523
 940.5880    1004.7992    1064.5971
1087.7009    1172.7121    1192.6255
1268.4769    1322.2559    1338.0124
1403.0610    1416.3325    1425.7093
1498.8568    1506.0006    1511.9173
1526.6702    3033.3054    3064.0834
3078.9226    3081.4436    3114.1325
3136.6054    3144.9493    3799.8074
Zero-point correction (Hartree): 0.116901

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C3H7O3H.ppm

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61718976
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.471528      1.200068      0.076782
  O      0.659295      0.770372     -0.682123
  O      1.604424      0.231110      0.202237
  O      1.439086     -1.163913      0.200737
  H      1.954912     -1.429593     -0.572742
  C     -1.288273      0.064517      0.661926
  H     -0.126387      1.887289      0.851004
  H     -1.051724      1.761983     -0.658113
  C     -1.849375     -0.869297     -0.401079
  H     -0.671464     -0.490003      1.369383
  H     -2.099552      0.516946      1.236924
  H     -1.042348     -1.325768     -0.971141
  H     -2.491527     -0.327037     -1.097064
  H     -2.439288     -1.666097      0.049168
Rotational constants (GHz):   5.2943200  2.6546700  2.1061400
Vibrational harmonic frequencies (cm-1):
 101.1924     130.3271     166.8101
 219.3024     278.6351     352.9284
 443.9886     487.9698     617.4122
 769.0125     879.6059     899.7920
 933.8904     982.6912    1015.9900
1098.0459    1125.6492    1192.1422
1291.3539    1314.3441    1382.2305
1404.2720    1419.9873    1422.4903
1482.3390    1486.0675    1502.5727
1509.4614    3062.4873    3064.4203
3070.4569    3106.9793    3119.7638
3134.3109    3150.6826    3794.9589
Zero-point correction (Hartree): 0.117131

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C3H7O3H.pmp

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-----
E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61444605
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.503919     -1.235265      0.118978
  O     -0.895891     -1.061729     -0.093601
  O     -1.330568      0.091909      0.574202

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O	-1.383949	1.127128	-0.373808
H	-2.237273	0.969123	-0.800240
C	1.397257	-0.183323	-0.522932
H	0.689186	-1.309690	1.193771
H	0.673174	-2.214928	-0.329002
C	1.646231	1.049164	0.340034
H	2.354363	-0.665421	-0.734593
H	0.965154	0.096012	-1.484657
H	2.079405	0.760312	1.298903
H	0.728495	1.597580	0.534798
H	2.346316	1.725097	-0.149796
Rotational constants (GHz): 4.8573900 2.9283900 2.1254500			
Vibrational harmonic frequencies (cm-1):			
98.9845	126.0725	173.2754	
227.3515	323.9656	349.9888	
397.0798	484.3859	598.3285	
757.6847	868.6439	921.2014	
938.3822	988.8667	1029.4760	
1110.0444	1133.2453	1168.4048	
1293.7373	1328.8798	1374.5594	
1413.2341	1420.9770	1426.7778	
1473.1766	1483.6106	1504.8902	
1511.6026	3057.4461	3063.1566	
3067.1543	3108.5603	3119.4310	
3129.6883	3170.8752	3795.4941	
Zero-point correction (Hartree): 0.117186			

C3H7O3H.ppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61653934

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.474005	0.906632	0.021763
O	0.896156	0.968284	-0.364475
O	1.644482	0.178633	0.520016
O	1.809518	-1.082416	-0.075973
H	2.558100	-0.931665	-0.669117
C	-1.124199	-0.445703	-0.191258
H	-0.561046	1.225225	1.063610
H	-0.938886	1.666114	-0.610181
C	-2.613267	-0.373112	0.125251
H	-0.963224	-0.757516	-1.224047
H	-0.637473	-1.184143	0.444729
H	-3.119170	0.345628	-0.521000
H	-2.779354	-0.065597	1.158639
H	-3.091371	-1.340954	-0.013716
Rotational constants (GHz): 7.2487100 1.9730800 1.6789900			
Vibrational harmonic frequencies (cm-1):			
92.4111	117.6707	142.7065	
234.7104	263.7185	342.9261	
398.4391	503.5064	614.5148	
759.9620	891.2366	897.7975	
931.2319	995.8951	1052.0384	
1085.9913	1141.1397	1202.1807	
1292.8343	1323.0082	1344.8823	
1414.0554	1421.5979	1426.8004	
1483.9059	1496.2505	1506.4229	
1513.1994	3056.0012	3059.8905	
3081.6953	3102.3805	3115.2650	
3139.0585	3142.4426	3791.9036	
Zero-point correction (Hartree): 0.117052			

C3H7O3H.pppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61631032

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.380838	-1.006715	0.351826
O	0.577103	-0.704056	-0.665850
O	1.129140	0.559538	-0.410691
O	2.157114	0.377225	0.528475
H	2.880160	0.042900	-0.020234
C	-1.750642	-0.423167	0.066498
H	-0.416982	-2.096502	0.360232
H	0.021391	-0.668585	1.308578
C	-1.782914	1.099465	0.032384
H	-2.108835	-0.827232	-0.882222

H	-2.425940	-0.793865	0.841724
H	-1.178285	1.485160	-0.786363
H	-1.389640	1.519694	0.958700
H	-2.802359	1.459274	-0.100140
Rotational constants (GHz):	6.5167700	2.2249400	1.9185200
Vibrational harmonic frequencies (cm-1):			
67.9566	115.4632		154.2903
262.7205	309.8353		365.8688
398.2863	544.6639		602.4158
782.0293	861.6025		910.2072
931.7405	979.0540		1023.4495
1100.2315	1123.5530		1184.4617
1298.3074	1314.9153		1382.5969
1407.4651	1422.0664		1423.6286
1480.3954	1487.4769		1502.1005
1511.1376	3057.5769		3067.3686
3073.8700	3096.2584		3125.5970
3135.7506	3147.9849		3786.7572
Zero-point correction (Hartree):	0.117187		

C3H7O3H.pppp

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -344.15030586
 E (CCSD/Aug-CC-pVTZ) (Hartree): -344.09428393
 T1 diagnostic: 0.014002
 E (MP2/Aug-CC-pVTZ) (Hartree): -344.05746262
 E (MP3/Aug-CC-pVTZ) (Hartree): -344.08543184
 E (RHF/Aug-CC-pVTZ) (Hartree): -342.78025312
 E (RM062X/Aug-CC-pVTZ) (Hartree): -344.61782901
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.317591	0.897982	-0.347289
O	-0.483264	-0.172535	-0.850714
O	-1.226107	-0.709304	0.209648
O	-2.339733	0.125499	0.401234
H	-2.938575	-0.168802	-0.298863
C	1.393581	0.428707	0.611879
H	0.753566	1.321356	-1.253947
H	-0.340273	1.641022	0.106019
C	2.340965	-0.582778	-0.019029
H	1.943515	1.311552	0.944665
H	0.916811	0.004348	1.495874
H	2.839068	-0.157991	-0.892000
H	1.797415	-1.468799	-0.343558
H	3.108486	-0.895426	0.687106
Rotational constants (GHz):	8.2933400	1.8918000	1.8440300
Vibrational harmonic frequencies (cm-1):			
43.0723	101.0695		181.2912
232.1875	279.8720		390.2341
414.3600	556.2491		598.5013
771.5105	881.2417		897.7187
931.9266	977.3811		1017.0843
1093.1729	1122.9560		1192.1589
1292.3724	1310.5926		1381.3744
1403.4608	1420.8833		1423.4097
1484.5277	1487.7562		1504.9894
1510.8223	3063.4416		3068.5862
3075.0353	3106.9813		3123.2553
3134.3216	3146.2244		3791.7692
Zero-point correction (Hartree):	0.117125		

C3H7O3H.pppt

E (RM062X/Aug-CC-pVTZ) (Hartree): -344.61748152
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.381775	0.383475	0.586810
O	-0.823222	0.959637	0.087506
O	-1.505514	-0.014150	-0.655003
O	-2.204734	-0.818333	0.260272
H	-2.982275	-0.277376	0.455624
C	1.398541	0.100382	-0.499873
H	0.750933	1.135698	1.286041
H	0.132787	-0.518041	1.151538
C	2.680553	-0.471588	0.092604
H	0.966352	-0.600275	-1.214196
H	1.605147	1.026785	-1.037757

H	2.484414	-1.406322	0.619227	
H	3.129347	0.223324	0.803847	
H	3.415846	-0.674637	-0.683772	
Rotational constants (GHz):		8.6978700	1.6910200	1.6206800
Vibrational harmonic frequencies (cm-1):				
78.7164		85.4037		167.8681
236.2473		275.0395		341.1238
391.2310		562.9043		597.6459
760.0181		884.9262		903.0348
925.7982		991.9810		1053.4579
1078.8885		1142.7064		1203.5649
1289.7184		1324.9510		1336.0613
1414.1208		1418.0705		1423.6082
1489.7257		1499.4954		1505.4630
1515.3964		3059.8795		3064.2487
3077.2646		3103.8694		3117.1993
3136.0083		3141.5785		3790.7001
Zero-point correction (Hartree): 0.117070				

C3H7O3H.pptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61749176

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.303498	0.565166	0.442251	
O	-0.391334	-0.456771	-0.272226	
O	-1.644155	-0.636870	0.322988	
O	-2.491665	0.367375	-0.175357	
H	-2.758246	0.003581	-1.030722	
C	1.670293	0.696185	-0.197636	
H	-0.265512	1.492846	0.369390	
H	0.381415	0.266217	1.490269	
C	2.518018	-0.561371	-0.049092	
H	1.540886	0.946556	-1.251955	
H	2.168888	1.546550	0.270438	
H	2.038390	-1.412284	-0.529453	
H	2.660005	-0.807567	1.004009	
H	3.500553	-0.425649	-0.498360	
Rotational constants (GHz):		10.8260000	1.6500600	1.5440100
Vibrational harmonic frequencies (cm-1):				
59.4502		102.0543		161.4532
201.1388		298.5073		346.4743
401.9670		477.0573		619.5992
763.1866		909.8249		932.7788
940.1118		974.4301		1033.7849
1096.4133		1155.1562		1185.0571
1269.3994		1311.1512		1376.4714
1410.8405		1421.0995		1421.6237
1482.6863		1500.1763		1510.7585
1527.4592		3058.4922		3066.3616
3070.0145		3105.6140		3116.4046
3135.6764		3149.0056		3794.3240
Zero-point correction (Hartree): 0.117066				

C3H7O3H.pptp

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61747868

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.343802	-0.717612	0.472886	
O	-0.438541	-0.290404	-0.641775	
O	-1.790311	-0.406867	-0.300711	
O	-2.135439	0.741466	0.432038	
H	-2.282873	1.393210	-0.266925	
C	1.796622	-0.521691	0.090720	
H	0.079132	-0.108378	1.339932	
H	0.116068	-1.764462	0.679461	
C	2.164214	0.943657	-0.108284	
H	2.403831	-0.959256	0.884835	
H	2.001974	-1.093174	-0.816057	
H	1.964669	1.517002	0.797959	
H	1.583426	1.382950	-0.917325	
H	3.220270	1.052421	-0.350221	
Rotational constants (GHz):		7.7942000	1.8447800	1.6822000
Vibrational harmonic frequencies (cm-1):				
53.8689		101.5834		170.5222
205.5706		298.8920		340.6356

407.1874	460.2171	625.7937
762.5574	908.6927	930.8264
938.5073	977.7510	1033.4372
1095.9155	1157.2285	1184.2780
1270.8501	1311.8672	1376.1365
1411.1126	1421.4422	1421.9246
1482.7932	1500.5987	1511.0916
1526.2901	3060.2138	3066.1871
3069.6280	3104.1711	3114.3913
3135.7896	3148.5925	3793.3587

Zero-point correction (Hartree): 0.117052

C3H7O3H.pptt

E(RM062X/Aug-CC-pVTZ) (Hartree): -344.61741459

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.366493	0.077471	0.314454
O	-0.692933	-0.741159	-0.174416
O	-1.880123	-0.345123	0.452090
O	-2.363936	0.776761	-0.242078
H	-2.802279	0.372402	-1.003299
C	1.634035	-0.378173	-0.376050
H	0.144707	1.121688	0.084116
H	0.437658	-0.044425	1.397708
C	2.832935	0.435253	0.096211
H	1.788798	-1.438043	-0.170002
H	1.506201	-0.275508	-1.454366
H	2.980366	0.326949	1.171103
H	2.694675	1.495610	-0.116916
H	3.745022	0.110183	-0.400803

Rotational constants (GHz): 11.3104300 1.4828100 1.4164700

Vibrational harmonic frequencies (cm-1):

80.2959	85.7372	163.7135
210.3116	238.8804	377.0483
394.1569	453.9305	613.5518
769.1786	912.6502	928.7492
939.7186	1003.9996	1061.7720
1083.1549	1169.6994	1194.9779
1269.8706	1318.9313	1337.1937
1415.8811	1421.2761	1423.8504
1498.8873	1505.9360	1512.8579
1530.8275	3056.3110	3064.0830
3075.4974	3097.7896	3116.0048
3136.2012	3143.0522	3791.3599

Zero-point correction (Hartree): 0.117092

C4H9O.pm

E(UM062X/Aug-CC-pVTZ) (Hartree): -232.96940661

Electronic state : 2-A

Cartesian coordinates (Angs):

C	1.305218	0.264210	0.293980
O	1.436472	-1.028862	-0.141226
C	0.151084	1.026035	-0.351547
H	1.263054	0.318968	1.391030
H	2.261490	0.729934	-0.004222
C	-1.206760	0.593507	0.195099
H	0.298080	2.093222	-0.174449
H	0.195749	0.859436	-1.429953
C	-1.506180	-0.882939	-0.032227
H	-1.245590	0.815836	1.264899
H	-1.982931	1.201361	-0.273350
H	-0.789500	-1.520401	0.488665
H	-1.450475	-1.132234	-1.092311
H	-2.501829	-1.140108	0.327674

Rotational constants (GHz): 7.5470300 3.8679100 2.8639100

Vibrational harmonic frequencies (cm-1):

105.6551	147.9298	249.3584
320.0858	367.2515	477.3945
772.5249	805.3108	861.3340
913.0865	950.0525	1049.2242
1072.6172	1097.1404	1123.8683
1173.6270	1240.3266	1298.8181
1340.9202	1367.9703	1378.9799
1413.8930	1420.7735	1473.7882
1487.4895	1502.6557	1506.8419

2942.0283	3002.4993	3050.2006
3055.8143	3060.8003	3087.5041
3108.2019	3122.4180	3134.5038

Zero-point correction (Hartree): 0.124121

C4H9O.pp

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E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -232.61662034
E (CCSD/Aug-CC-pVTZ) (Hartree): -232.57933627
  T1 diagnostic: 0.014945
E (MP2/Aug-CC-pVTZ) (Hartree): -232.52181191
E (MP3/Aug-CC-pVTZ) (Hartree): -232.57373170
E (PMP2/Aug-CC-pVTZ) (Hartree): -232.52428113
E (PMP3/Aug-CC-pVTZ) (Hartree): -232.57522892
E (PUHF/Aug-CC-pVTZ) (Hartree): -231.61927472
E (UHF/Aug-CC-pVTZ) (Hartree): -231.61524039
E (UM062X/Aug-CC-pVTZ) (Hartree): -232.96901063
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      1.232568      0.028182      0.520953
  O      1.735762     -0.723722     -0.505311
  C      0.138747      1.009269      0.116646
  H      0.843164     -0.718147      1.237265
  H      2.053136      0.521406      1.060713
  C     -1.041314      0.345140     -0.586054
  H     -0.202575      1.529407      1.016160
  H      0.582416      1.762813     -0.536692
  C     -1.794038     -0.643653      0.297652
  H     -1.727029      1.122875     -0.925165
  H     -0.677545     -0.163383     -1.480012
  H     -2.111374     -0.172382      1.229851
  H     -1.178365     -1.506972      0.550917
  H     -2.683702     -1.019476     -0.205735
Rotational constants (GHz):      8.5216600      3.1279500      2.8395100
Vibrational harmonic frequencies (cm-1):
  45.4801      160.0919      261.8935
  278.5835      388.1302      517.6745
  587.6126      762.7656      849.6906
  878.9048      955.4685     1038.0397
 1047.1881     1092.1234     1130.8602
 1181.9876     1258.4628     1310.2869
 1341.8900     1372.7355     1380.2589
 1399.5976     1417.0404     1480.9883
 1492.7656     1504.2754     1513.5175
 2938.5720     2997.7211     3052.4528
 3057.2726     3070.1372     3097.2947
 3104.2304     3126.9667     3134.6349
Zero-point correction (Hartree): 0.123540

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C4H9O.pt

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E (UM062X/Aug-CC-pVTZ) (Hartree): -232.96966695
Electronic state : 2-A
Cartesian coordinates (Angs):
  C      1.490917      0.414800      0.226991
  O      2.020315     -0.751268     -0.259806
  C      0.060976      0.691628     -0.204705
  H      1.593109      0.411883      1.324213
  H      2.179069      1.209487     -0.108426
  C     -0.909314     -0.350870      0.336290
  H     -0.230644      1.688175      0.138322
  H      0.022328      0.702018     -1.296682
  C     -2.337924     -0.116200     -0.134338
  H     -0.569643     -1.340098      0.022223
  H     -0.872262     -0.341063      1.429160
  H     -2.396834     -0.152681     -1.222847
  H     -2.696667      0.863840      0.183800
  H     -3.018901     -0.867556      0.263261
Rotational constants (GHz):     13.4139400      2.4197800      2.2485300
Vibrational harmonic frequencies (cm-1):
  i179.2370      102.0914      136.7784
  242.7549      250.5012      354.2786
  541.5340      745.8846      863.5530
  866.5408      969.9209     1017.0127
 1064.8460     1095.0823     1139.0106
 1210.1307     1265.2785     1321.0560
 1329.9209     1367.1781     1397.9450

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1404.3109	1414.5090	1477.6398
1496.5591	1503.4102	1511.2086
2951.9330	2975.2727	3046.4825
3053.9953	3058.5410	3080.9285
3100.8480	3125.1578	3134.5149

Zero-point correction (Hartree): 0.122148

C4H9O.tp

E(UM062X/Aug-CC-pVTZ) (Hartree): -232.96843310

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-1.079646	-0.333061	0.273893
O	-2.379649	-0.210016	-0.130103
C	-0.147804	0.745733	-0.265315
H	-1.012975	-0.419635	1.369123
H	-0.781529	-1.325054	-0.112401
C	1.277039	0.607034	0.262730
H	-0.155553	0.700510	-1.356356
H	-0.557581	1.716377	0.018188
C	1.954003	-0.692845	-0.159319
H	1.865629	1.453719	-0.092675
H	1.266786	0.678137	1.353584
H	1.924883	-0.809338	-1.244029
H	1.468276	-1.563655	0.282074
H	2.997699	-0.712102	0.151372

Rotational constants (GHz): 12.3503700 2.5009600 2.2748000

Vibrational harmonic frequencies (cm-1):

90.7415	118.5115	227.6909
286.5456	339.0768	466.2071
669.8976	763.6677	873.0169
892.3175	968.2728	1030.9235
1064.7931	1092.4098	1121.0963
1198.2400	1252.4382	1298.0482
1327.7120	1363.7136	1379.5722
1394.8949	1416.9614	1490.3846
1493.8298	1506.0950	1512.7941
2936.6385	2985.0036	3053.6842
3059.7124	3064.5547	3094.3437
3110.8234	3126.1507	3135.3359

Zero-point correction (Hartree): 0.123491

C4H9O.tt

E(UM062X/Aug-CC-pVTZ) (Hartree): -232.96848395

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-1.403376	0.478671	0.000040
O	-2.444742	-0.407888	-0.000073
C	-0.107497	-0.361807	0.000023
H	-1.407337	1.106273	-0.899228
H	-1.407379	1.105806	0.899661
C	1.126528	0.532010	-0.000040
H	-0.110991	-1.006300	0.879937
H	-0.110978	-1.006343	-0.879865
C	2.412580	-0.284458	0.000027
H	1.101788	1.183660	-0.876044
H	1.101810	1.183749	0.875905
H	2.465583	-0.925066	-0.880847
H	2.465402	-0.925143	0.880824
H	3.290633	0.359975	-0.000059

Rotational constants (GHz): 18.8829000 2.1083700 1.9907600

Vibrational harmonic frequencies (cm-1):

105.5788	121.7060	195.5663
247.1036	391.0754	419.1536
726.2195	775.2869	899.4704
910.6939	969.7792	1055.7982
1089.4320	1093.7894	1152.7438
1237.1538	1277.8599	1292.3250
1318.0728	1326.2306	1383.7577
1415.1743	1492.4936	1498.5135
1503.2048	1511.6997	1538.2091
2998.4834	3045.9689	3055.8425
3061.0413	3075.7929	3087.3430
3122.7004	3132.7250	3136.4540

Zero-point correction (Hartree): 0.124535

C4H9OO.pmm

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13735238
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.803664	0.783254	0.612950
O	-1.696381	-0.005192	-0.204261
O	-1.413420	-1.271732	-0.149488
C	0.412663	1.210078	-0.186827
H	-1.398340	1.643187	0.916452
H	-0.549871	0.180810	1.482645
C	1.295977	0.060947	-0.667342
H	0.073464	1.803174	-1.037918
H	0.994912	1.878353	0.454003
C	1.893581	-0.763782	0.466439
H	0.720403	-0.588143	-1.329166
H	2.098068	0.486665	-1.272417
H	1.122526	-1.316554	1.001513
H	2.417013	-0.125460	1.181064
H	2.608893	-1.489620	0.082490

Rotational constants (GHz): 5.2779700 2.5676100 2.0673200
 Vibrational harmonic frequencies (cm-1):

89.2740	103.7986	159.4462
258.0005	268.8748	389.4892
466.7629	554.1194	751.2674
827.8944	857.6412	935.0415
997.1192	1003.6242	1092.2008
1133.9149	1155.9796	1242.6300
1262.4512	1309.9122	1334.9995
1370.1317	1394.0530	1401.8417
1416.5820	1474.6456	1488.6773
1495.7759	1504.3919	1519.8349
3053.5004	3057.5091	3068.1740
3096.3890	3099.8055	3106.9965
3128.0379	3140.3711	3159.2103

Zero-point correction (Hartree): 0.130244

C4H9OO.pmp

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13463369
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	1.027179	0.980485	-0.046801
O	1.411581	-0.305529	0.488180
O	1.387250	-1.237427	-0.415619
C	-0.450142	1.253225	0.159959
H	1.643133	1.699246	0.491964
H	1.295348	0.971295	-1.101911
C	-1.389343	0.253915	-0.524550
H	-0.662722	1.293827	1.230694
H	-0.621420	2.259289	-0.229645
C	-1.736835	-0.953153	0.342209
H	-2.312366	0.771159	-0.789707
H	-0.940171	-0.080174	-1.462407
H	-2.226316	-0.631416	1.262692
H	-0.852167	-1.524800	0.614567
H	-2.419121	-1.621614	-0.181639

Rotational constants (GHz): 4.8806000 2.8125100 2.0682000
 Vibrational harmonic frequencies (cm-1):

83.2537	103.3885	144.5282
220.5800	291.0159	360.7208
458.4204	538.7989	764.7634
823.9301	864.7793	937.4414
993.5507	1014.0807	1106.9264
1113.5679	1175.3543	1249.7586
1266.7229	1306.5836	1336.0615
1370.3802	1397.6313	1399.5332
1420.8008	1478.4581	1485.0981
1494.0236	1507.5114	1511.1193
3058.1874	3061.3978	3065.4349
3089.2747	3098.4572	3101.4512
3129.6052	3152.9203	3156.9878

Zero-point correction (Hartree): 0.130157

C4H9OO.pmt

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13727080

Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-1.015483	0.950127	0.292993
O	-1.770739	-0.015478	-0.471582
O	-1.833464	-1.168168	0.123642
C	0.446960	0.916615	-0.101447
H	-1.474368	1.908195	0.054098
H	-1.166312	0.710718	1.344553
C	1.152435	-0.389854	0.240128
H	0.529403	1.117783	-1.172388
H	0.939547	1.747398	0.411788
C	2.629028	-0.345890	-0.131116
H	1.039099	-0.591232	1.307897
H	0.663352	-1.214780	-0.279322
H	3.143015	0.455280	0.402002
H	2.755054	-0.166866	-1.199783
H	3.127191	-1.283317	0.111333

Rotational constants (GHz): 7.1533100 1.9208500 1.6382100
 Vibrational harmonic frequencies (cm-1):

83.8288	104.2568	125.5466
238.9620	248.8776	334.2141
476.6225	545.6121	741.2515
837.5663	855.0855	942.6823
984.6339	1037.4325	1080.4062
1135.0729	1179.4183	1247.6070
1266.8928	1312.4262	1334.4106
1349.2884	1395.4330	1411.1788
1415.4926	1475.0783	1486.2136
1494.5045	1504.4726	1511.1715
3050.1484	3057.6783	3064.4163
3084.4285	3094.4492	3106.3306
3127.7627	3137.7051	3153.6111

Zero-point correction (Hartree): 0.129929

C4H9OO.ppm

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13635841
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.726902	0.897304	-0.515924
O	-1.307168	-0.430609	-0.506870
O	-1.929728	-0.668890	0.604983
C	0.409317	1.031630	0.478364
H	-0.392012	1.028514	-1.545076
H	-1.538272	1.589940	-0.298297
C	1.709327	0.350832	0.059474
H	0.586536	2.099651	0.619623
H	0.059654	0.641956	1.436820
C	1.598651	-1.161237	-0.105270
H	2.060816	0.797640	-0.874466
H	2.467832	0.577744	0.810525
H	0.948372	-1.428746	-0.937008
H	1.182346	-1.619932	0.792769
H	2.577541	-1.601942	-0.289658

Rotational constants (GHz): 5.5721400 2.4420600 2.0254800
 Vibrational harmonic frequencies (cm-1):

56.2325	101.6554	168.9286
265.1519	313.1195	320.2154
464.4452	554.6189	782.1816
817.7829	857.0024	937.0200
965.3634	1014.3154	1098.5324
1116.1370	1179.3603	1238.2770
1280.7831	1297.0816	1328.3260
1377.7613	1390.0671	1405.1042
1422.6217	1476.5915	1485.9974
1496.3902	1504.7481	1511.3440
3049.8688	3063.8454	3065.3029
3085.9072	3090.1983	3110.0350
3131.6864	3141.3848	3145.8613

Zero-point correction (Hartree): 0.130109

C4H9OO.ppp

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13732586
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.630167	0.396789	0.896504
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O	1.328829	-0.697664	0.258398
O	2.141492	-0.270171	-0.658434
C	-0.313702	1.082230	-0.070486
H	0.106961	-0.077501	1.724679
H	1.385309	1.080377	1.281225
C	-1.301217	0.134319	-0.747920
H	-0.855103	1.843581	0.497361
H	0.280934	1.601977	-0.821716
C	-2.156319	-0.660144	0.232319
H	-1.944935	0.725659	-1.400263
H	-0.752221	-0.551436	-1.395173
H	-2.650417	0.000650	0.947454
H	-1.558267	-1.377401	0.794833
H	-2.928401	-1.222387	-0.290611

Rotational constants (GHz): 6.4979000 2.0675800 2.0225900

Vibrational harmonic frequencies (cm-1):

43.7878	96.3241	183.5446
237.9648	287.4996	376.4427
465.6113	588.4700	732.7572
828.7773	853.9559	940.4148
981.2021	1014.1141	1089.5103
1131.9206	1163.6287	1240.2821
1269.2829	1301.7972	1325.8623
1372.6043	1391.7789	1406.9089
1418.3820	1477.9506	1492.0526
1497.1716	1505.5947	1518.4691
3056.2340	3060.7143	3071.3529
3096.8379	3102.6454	3115.7096
3127.0950	3136.3010	3155.4660

Zero-point correction (Hartree): 0.130212

C4H9OO.ppt

E (CCSD(T)/Aug-CC-pVTZ) (Hartree): -307.69397198

E (CCSD/Aug-CC-pVTZ) (Hartree): -307.64388997

T1 diagnostic: 0.021375

E (MP2/Aug-CC-pVTZ) (Hartree): -307.58734458

E (MP3/Aug-CC-pVTZ) (Hartree): -307.63179376

E (PMP2/Aug-CC-pVTZ) (Hartree): -307.59051018

E (PMP3/Aug-CC-pVTZ) (Hartree): -307.63365996

E (PUHF/Aug-CC-pVTZ) (Hartree): -306.43502262

E (UHF/Aug-CC-pVTZ) (Hartree): -306.42986636

E (UM062X/Aug-CC-pVTZ) (Hartree): -308.13785551

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.969806	0.976091	-0.010699
O	-1.678391	-0.158787	-0.563645
O	-2.070932	-0.970234	0.369321
C	0.371674	0.557491	0.549855
H	-0.866524	1.655521	-0.856209
H	-1.616023	1.416493	0.746740
C	1.310726	-0.021676	-0.501389
H	0.826885	1.435826	1.014649
H	0.199411	-0.169875	1.345755
C	2.649491	-0.432916	0.096311
H	0.834840	-0.883467	-0.972269
H	1.467498	0.717936	-1.290801
H	2.511203	-1.190656	0.868346
H	3.150119	0.420844	0.555274
H	3.314661	-0.844387	-0.661361

Rotational constants (GHz): 7.7196900 1.7590600 1.6400100

Vibrational harmonic frequencies (cm-1):

68.4681	84.6561	163.9605
240.1226	255.9331	320.6898
468.9442	571.9691	741.5799
835.8285	857.9939	937.0943
976.9846	1043.9490	1078.5544
1139.3139	1180.3900	1242.6077
1276.6441	1304.4422	1334.6448
1340.0768	1399.0529	1409.3103
1415.5210	1478.4847	1491.1016
1497.1717	1504.4977	1512.3039
3052.0825	3058.7463	3062.0355
3086.8326	3091.5044	3109.2922
3127.3791	3137.4129	3148.8565

Zero-point correction (Hartree): 0.129961

C4H9OO.ptm

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13667857
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.512341	-0.542598	0.237996
O	1.863674	-0.563646	-0.272810
O	2.565010	0.419752	0.201081
C	-0.279942	0.586955	-0.386630
H	0.119078	-1.523901	-0.019937
H	0.575923	-0.440086	1.321738
C	-1.683202	0.702214	0.203983
H	0.274150	1.511546	-0.222447
H	-0.339704	0.424715	-1.465233
C	-2.544726	-0.535584	-0.024960
H	-1.607153	0.905899	1.274810
H	-2.171835	1.570284	-0.239594
H	-2.157249	-1.403086	0.509750
H	-2.584411	-0.788465	-1.085795
H	-3.565093	-0.371676	0.318211

Rotational constants (GHz): 10.5200800 1.5828000 1.4721300
 Vibrational harmonic frequencies (cm-1):

58.9501	104.2109	133.0117
228.7318	290.4080	317.4511
448.5264	572.5540	750.3042
804.6997	897.3512	953.8290
970.3341	1016.3454	1097.3443
1134.1296	1183.4637	1241.9787
1279.7473	1299.6867	1329.9553
1351.8393	1378.6070	1413.4775
1419.3076	1485.5942	1494.9750
1502.3686	1508.3204	1513.7996
3057.7335	3061.2722	3065.3792
3087.4620	3098.2368	3115.1628
3128.5607	3137.6078	3154.6229

Zero-point correction (Hartree): 0.130055

C4H9OO.ptp

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13651651
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.549392	0.060767	0.667246
O	-1.952884	0.228170	0.369649
O	-2.339252	-0.590925	-0.559742
C	0.302358	0.645386	-0.440117
H	-0.407510	0.589552	1.609760
H	-0.379381	-1.004859	0.808863
C	1.793492	0.593337	-0.114687
H	0.097070	0.092074	-1.358468
H	-0.009096	1.678347	-0.603528
C	2.334580	-0.824158	0.043716
H	2.335329	1.099030	-0.914596
H	1.986914	1.166344	0.795729
H	2.094836	-1.428984	-0.832082
H	1.915494	-1.323645	0.917122
H	3.417205	-0.817811	0.160993

Rotational constants (GHz): 8.6120700 1.6350100 1.5750900
 Vibrational harmonic frequencies (cm-1):

57.5478	105.7256	124.7243
228.7530	285.2157	326.1158
433.2798	579.3761	754.3897
805.2050	896.6531	944.6273
980.2616	1010.7755	1097.3660
1134.6715	1186.8021	1241.5830
1288.5489	1289.7305	1335.4020
1351.2766	1378.3975	1411.2553
1420.6453	1486.5997	1494.2188
1502.5236	1508.6258	1513.9334
3055.2022	3062.5645	3066.3931
3091.1253	3097.1235	3111.2106
3130.2995	3137.8122	3154.1198

Zero-point correction (Hartree): 0.130038

C4H9OO.ptt

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13747483

Electronic state : 2-A
 Cartesian coordinates (Angs):

C	-0.819433	0.762890	0.096877
O	-2.061030	0.211619	-0.392771
O	-2.437395	-0.807801	0.316541
C	0.346709	-0.139337	-0.241490
H	-0.742366	1.731580	-0.395523
H	-0.928170	0.901253	1.172332
C	1.664374	0.438232	0.261960
H	0.168357	-1.118025	0.207636
H	0.388255	-0.279485	-1.323967
C	2.847290	-0.460686	-0.073315
H	1.818983	1.428250	-0.174425
H	1.605707	0.582147	1.343503
H	2.937496	-0.595756	-1.151639
H	2.722470	-1.446599	0.375391
H	3.783021	-0.040502	0.292328

Rotational constants (GHz): 11.0537100 1.4351800 1.3551900
 Vibrational harmonic frequencies (cm-1):

84.5287	94.4792	136.2753
190.3500	248.5360	360.4829
408.3097	569.1493	742.7447
808.8675	920.5997	945.3710
977.9563	1052.2429	1084.9703
1141.6740	1197.7605	1246.3703
1281.0084	1296.8591	1330.3230
1335.4903	1384.7077	1414.5276
1417.2732	1489.2801	1493.6631
1502.9857	1504.3532	1515.7232
3049.2026	3061.9826	3065.0328
3079.8683	3088.5468	3110.4395
3130.4169	3138.7457	3149.2077

Zero-point correction (Hartree): 0.129970

C4H9OO.tpm

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13559082
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.662789	0.861833	0.295169
O	1.263249	-0.272135	-0.377623
O	2.404937	-0.587601	0.148462
C	-0.700247	1.114513	-0.313735
H	0.611176	0.614562	1.356281
H	1.343886	1.699698	0.153016
C	-1.809726	0.210505	0.219149
H	-0.957251	2.157140	-0.120277
H	-0.613165	1.010947	-1.398318
C	-1.572593	-1.275783	-0.023519
H	-1.926756	0.392371	1.290617
H	-2.749887	0.509930	-0.246753
H	-0.699286	-1.636531	0.518661
H	-1.403427	-1.475257	-1.082249
H	-2.432116	-1.861387	0.299926

Rotational constants (GHz): 6.2568800 2.1654600 1.7487500
 Vibrational harmonic frequencies (cm-1):

65.2461	87.6772	138.1798
262.7221	292.3398	325.9958
416.2221	541.5219	775.1424
816.5965	859.2368	956.4738
981.0709	1016.0417	1112.2654
1128.8216	1166.1109	1246.6539
1284.4061	1297.3548	1313.0029
1376.6996	1388.6437	1412.3596
1425.5271	1474.5154	1489.8481
1503.0892	1504.8117	1510.9113
3053.2950	3062.4111	3066.0865
3078.8674	3093.3442	3108.4122
3134.4760	3135.6757	3141.4104

Zero-point correction (Hartree): 0.129955

C4H9OO.tpp

 E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13661044
 Electronic state : 2-A
 Cartesian coordinates (Angs):

C	0.648812	0.559466	0.616123
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O	1.368865	-0.073465	-0.466687
O	2.427691	-0.689753	-0.041683
C	-0.620713	1.147664	0.043493
H	0.461707	-0.206683	1.367009
H	1.305169	1.320049	1.036953
C	-1.541219	0.119332	-0.613673
H	-1.144490	1.641369	0.865792
H	-0.356290	1.924387	-0.675853
C	-1.972697	-0.999753	0.327192
H	-2.422559	0.642497	-0.986819
H	-1.041084	-0.306314	-1.484474
H	-2.407820	-0.596228	1.243503
H	-1.133067	-1.636424	0.606208
H	-2.719110	-1.637159	-0.144169

Rotational constants (GHz): 6.5685500 1.9706200 1.7605900

Vibrational harmonic frequencies (cm-1):

43.7619	79.8287	155.8301
235.2641	290.8957	353.8557
436.5540	552.0840	737.7258
831.2626	857.2494	965.2672
982.5479	1011.7681	1101.8886
1133.5144	1165.2264	1238.4069
1275.0102	1298.6574	1323.5876
1369.6816	1389.9503	1408.7877
1422.2443	1476.6846	1495.5934
1500.6503	1506.3078	1521.7503
3058.3116	3061.8382	3072.2568
3090.4129	3100.8344	3109.1328
3129.0019	3137.1466	3144.9144

Zero-point correction (Hartree): 0.130005

C4H9OO.tpt

E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13724148

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.885659	0.776259	0.237124
O	1.517300	-0.390144	-0.341034
O	2.744768	-0.516104	0.056503
C	-0.556638	0.785073	-0.210797
H	0.985980	0.690430	1.319341
H	1.442234	1.645031	-0.111761
C	-1.368917	-0.377700	0.348317
H	-0.998358	1.732789	0.106242
H	-0.588922	0.774097	-1.303024
C	-2.816451	-0.340938	-0.122205
H	-0.904076	-1.318213	0.048945
H	-1.331596	-0.345173	1.440109
H	-2.871439	-0.399151	-1.209931
H	-3.302906	0.585915	0.185298
H	-3.389383	-1.171896	0.286392

Rotational constants (GHz): 10.8010600 1.5007500 1.4049100

Vibrational harmonic frequencies (cm-1):

68.9650	82.2853	131.5826
246.5964	258.5671	313.3822
393.3440	577.3883	735.5542
834.5015	854.7245	965.1405
973.9729	1051.4360	1088.6766
1149.0083	1171.9735	1247.3351
1281.2194	1298.2991	1329.5103
1339.8078	1396.9202	1414.7808
1416.6391	1478.0666	1497.0672
1502.6554	1505.2975	1512.4964
3053.4393	3058.5703	3063.2651
3080.8705	3090.0167	3107.2890
3127.8888	3137.7643	3139.3142

Zero-point correction (Hartree): 0.129800

C4H9OO.ttp

E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13603979

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.552084	0.165782	0.214748
O	1.841219	-0.322872	-0.218311
O	2.792081	0.505711	0.082867
C	-0.488404	-0.839437	-0.222718

H	0.591960	0.270656	1.300075
H	0.415702	1.147015	-0.236757
C	-1.878680	-0.497947	0.309866
H	-0.507398	-0.881451	-1.313853
H	-0.186340	-1.825753	0.132568
C	-2.405748	0.846260	-0.181536
H	-2.565501	-1.288894	0.007319
H	-1.858763	-0.508800	1.402301
H	-2.375924	0.898691	-1.271106
H	-1.818705	1.677960	0.208108
H	-3.436942	0.999913	0.132738
Rotational constants (GHz): 10.3201600 1.4935700 1.3814100			
Vibrational harmonic frequencies (cm-1):			
73.3897	87.6434	122.3747	
187.7827	278.8660	316.7421	
459.8329	515.2917	755.1723	
803.3828	897.4884	958.4415	
1002.7404	1021.9598	1100.3602	
1153.8309	1171.1461	1238.6561	
1289.6779	1300.1795	1314.9411	
1348.8301	1380.0212	1416.7589	
1424.6612	1492.9313	1496.7015	
1509.0622	1510.6163	1513.7766	
3058.2336	3061.8281	3065.1608	
3080.1194	3099.3094	3107.6570	
3129.2556	3137.2699	3144.4622	
Zero-point correction (Hartree): 0.129916			

C4H900.ttt

E(UM062X/Aug-CC-pVTZ) (Hartree): -308.13687328

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.785477	0.426913	0.000042
O	-1.890539	-0.503382	0.000031
O	-3.032372	0.111378	-0.000088
C	0.496021	-0.371147	0.000075
H	-0.886487	1.050205	-0.888668
H	-0.886518	1.050255	0.888719
C	1.719038	0.539447	0.000026
H	0.515393	-1.020071	0.878212
H	0.515430	-1.020140	-0.878013
C	3.020551	-0.251192	-0.000071
H	1.683998	1.192629	-0.875154
H	1.684107	1.192567	0.875241
H	3.084963	-0.890773	-0.880945
H	3.084792	-0.891345	0.880407
H	3.886815	0.408577	0.000228
Rotational constants (GHz): 18.3644900 1.2438800 1.1995600			
Vibrational harmonic frequencies (cm-1):			
62.4979	101.8897	125.0976	
144.8007	249.7679	344.4346	
379.6919	548.7180	742.1329	
806.6381	917.2618	950.1510	
1014.9600	1059.6037	1091.3577	
1160.8259	1174.7365	1246.3174	
1291.6680	1299.2775	1312.8802	
1331.5735	1385.0031	1417.2984	
1421.9386	1493.8265	1498.7119	
1504.8041	1506.0439	1517.5319	
3050.3816	3060.8537	3064.1930	
3079.8533	3079.9183	3104.6987	
3129.1126	3137.2575	3138.3633	
Zero-point correction (Hartree): 0.129733			

C4H903H.pmmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92061138

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.043144	1.272219	0.217603
O	0.923468	0.713666	-0.751249
O	2.022114	0.154748	-0.071847
O	1.886791	-1.238382	-0.115631
H	1.374039	-1.433262	0.681038
C	-0.686744	0.237563	1.057046
H	0.600846	1.967085	0.847983

H	-0.654944	1.848484	-0.390295
C	-1.450642	-0.805972	0.243309
H	0.024417	-0.243013	1.735957
H	-1.382700	0.780798	1.702617
C	-2.506853	-0.195605	-0.671307
H	-0.748380	-1.383718	-0.359465
H	-1.925943	-1.503210	0.935124
H	-2.051004	0.385042	-1.472788
H	-3.175362	0.463359	-0.113777
H	-3.113372	-0.971048	-1.136485
Rotational constants (GHz):			
	4.2790700	1.6019000	1.4381200
Vibrational harmonic frequencies (cm-1):			
55.2991	100.2751		117.3583
183.2099	220.3016		283.4937
352.2191	388.5086		465.3598
518.6952	606.8160		736.8453
828.5053	860.3796		920.6067
966.2585	974.7624		1013.9616
1046.5342	1109.6217		1139.0241
1167.4940	1260.5629		1287.0637
1329.6563	1373.3932		1392.3069
1408.1696	1415.1289		1417.9460
1484.6007	1495.0346		1496.6102
1506.9018	1518.0272		3041.2594
3057.9547	3066.2299		3072.2620
3078.5462	3105.2010		3124.4549
3130.2694	3139.9264		3785.3734
Zero-point correction (Hartree): 0.145899			

C4H9O3H.pmmmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91853797

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.142768	1.457430	-0.203416
O	1.008929	0.513959	-0.824774
O	1.881109	0.027797	0.176291
O	1.627167	-1.336590	0.317867
H	0.845328	-1.360510	0.888157
C	-0.898640	0.867958	0.733584
H	0.753453	2.199361	0.314913
H	-0.339110	1.944616	-1.053580
C	-1.999015	0.048458	0.058962
H	-0.398843	0.283844	1.514021
H	-1.352769	1.714530	1.254014
C	-1.578985	-1.349224	-0.382648
H	-2.839243	-0.037812	0.749996
H	-2.370767	0.608569	-0.802944
H	-1.278365	-1.950218	0.480146
H	-0.744838	-1.321382	-1.080431
H	-2.409254	-1.870059	-0.858263
Rotational constants (GHz):			
	3.5300800	1.9553600	1.4878000
Vibrational harmonic frequencies (cm-1):			
67.6411	94.3992		122.2134
172.8945	261.0187		294.5107
353.1680	359.5026		440.6856
515.5458	557.0499		768.2318
821.6994	856.6810		916.8036
961.7546	974.4616		1024.9152
1058.3820	1116.2245		1123.8368
1187.0267	1245.4005		1304.4265
1329.2838	1378.5676		1390.2420
1414.5576	1416.6625		1427.7361
1481.9648	1490.1682		1496.6464
1508.0102	1515.0198		3037.8688
3046.1294	3054.2282		3061.8582
3086.1931	3090.7632		3112.6955
3118.2886	3158.3385		3773.6359
Zero-point correction (Hartree): 0.145774			

C4H9O3H.pmmmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92108974

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.571011	-1.420669	0.099110
O	-1.441548	-0.557583	-0.625125

O	-1.957810	0.395178	0.272510
O	-1.338290	1.619017	-0.010563
H	-0.547303	1.598970	0.546342
C	0.691121	-0.742085	0.598206
H	-1.125567	-1.880318	0.919353
H	-0.331620	-2.192311	-0.634938
C	1.530380	-0.117666	-0.510493
H	0.426265	0.005261	1.354404
H	1.281755	-1.490506	1.133433
C	2.733238	0.639882	0.035731
H	1.864642	-0.908584	-1.186119
H	0.904942	0.548380	-1.106925
H	3.373557	-0.015089	0.628228
H	2.416374	1.460668	0.682349
H	3.335771	1.063864	-0.766022
Rotational constants (GHz):			
	3.9940900	1.6316800	1.3001600
Vibrational harmonic frequencies (cm-1):			
56.1592	112.9927		118.9670
187.4382	237.4326		263.3416
321.5414	351.9779		454.4439
517.1692	607.5974		747.5282
835.3648	859.8164		916.9689
963.8241	979.3647		1014.3512
1063.9542	1106.6273		1141.8942
1186.2412	1259.4423		1291.1086
1328.0987	1341.5195		1403.6240
1404.9801	1414.4408		1418.3868
1485.9294	1495.6632		1501.8054
1504.4989	1517.5818		3033.1003
3052.6335	3061.6860		3062.8526
3075.7100	3099.0440		3115.4470
3121.2097	3136.7641		3780.1055
Zero-point correction (Hartree): 0.145690			

C4H9O3H.pmmppm

Cartesian coordinates (Angs):

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.420000
O	1.357953	0.000000	1.835168
O	1.749388	1.338827	1.954842
H	2.083178	1.531689	1.064736
C	0.714189	1.237012	-0.548303
H	0.521186	-0.902721	-0.318685
H	-1.042372	0.000000	-0.318685
C	2.169386	1.283464	-0.078044
H	0.676172	1.171164	-1.635648
H	0.174557	2.107784	-0.175940
C	2.250851	1.331660	1.449025
H	2.652988	0.379543	-0.448391
H	2.613110	2.183712	-0.503206
H	1.767439	0.428968	1.822601
H	1.727561	2.233136	1.767786
H	3.308458	1.362994	1.710913

C4H9O3H.pmmpp

Cartesian coordinates (Angs):

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.420000
O	1.357953	0.000000	1.835168
O	1.749388	1.338827	1.954842
H	2.083178	1.531689	1.064736
C	0.714189	1.237012	-0.548303
H	0.521186	-0.902721	-0.318685
H	-1.042372	0.000000	-0.318685
C	2.169386	1.283464	-0.078044
H	0.676172	1.171164	-1.635648
H	0.174557	2.107784	-0.175940
C	2.938221	0.048197	-0.551234
H	2.613110	2.183712	-0.503206
H	2.151374	1.316163	1.011316
H	2.898792	0.046202	-1.640518
H	2.437056	-0.821347	-0.125996
H	3.959238	0.147850	-0.182869

C4H9O3H.pmmpt

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Cartesian coordinates (Angs):
  C      0.000000      0.000000      0.000000
  O      0.000000      0.000000      1.420000
  O      1.357953      0.000000      1.835168
  O      1.749388      1.338827      1.954842
  H      2.083178      1.531689      1.064736
  C      0.714189      1.237012     -0.548303
  H      0.521186     -0.902721     -0.318685
  H      -1.042372      0.000000     -0.318685
  C      2.169386      1.283464     -0.078044
  H      0.676172      1.171164     -1.635648
  H      0.174557      2.107784     -0.175940
  C      2.949561      2.373261     -0.815995
  H      2.152254      1.496692      0.990759
  H      2.603954      0.306446     -0.289437
  H      2.457259      3.320932     -0.597688
  H      2.908959      2.130686     -1.877884
  H      3.969975      2.349148     -0.433537

C4H9O3H.pmmtm
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E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91949141
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.018417      0.888582     -0.238118
  O      1.390113      0.945119     -0.422682
  O      1.996028      0.232200      0.628623
  O      2.459418     -0.978956      0.101033
  H      1.689219     -1.559279      0.175000
  C      -0.601993     -0.505708     -0.395607
  H      -0.268152      1.321232      0.732243
  H      -0.396330      1.551476     -1.019553
  C      -2.125623     -0.489799     -0.510150
  H      -0.166230     -0.962823     -1.286368
  H      -0.323787     -1.114122      0.471580
  C      -2.822013      0.089701      0.717201
  H      -2.409436      0.080053     -1.398250
  H      -2.473572     -1.510027     -0.675740
  H      -2.602872      1.149668      0.843571
  H      -2.501914     -0.426283      1.624026
  H      -3.903126     -0.013458      0.637741

Rotational constants (GHz):      5.6461700      1.2075700      1.1323700
Vibrational harmonic frequencies (cm-1):
  60.1147      103.3803      121.4081
  143.4752      230.1511      287.1201
  310.5591      354.5332      431.3041
  533.3086      584.8340      760.6825
  813.6526      899.9872      914.2989
  970.2604      985.5107     1011.2182
  1076.8326     1104.0473     1135.3412
  1198.4368     1268.6552     1287.6920
  1327.9038     1349.8362     1377.9304
  1417.2885     1422.1707     1426.2570
  1486.4777     1495.0994     1503.0973
  1512.0733     1513.7504     3030.7070
  3057.3014     3062.4477     3066.2558
  3090.9600     3097.7604     3118.0531
  3129.8298     3139.9543     3788.0031

Zero-point correction (Hartree): 0.145803

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C4H9O3H.pmmtp
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E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91949874
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      -0.025460      0.851810      0.224483
  O      1.292808      1.017695     -0.279679
  O      2.151342      0.170173      0.446312
  O      2.517974     -0.877322     -0.405765
  H      1.794664     -1.510923     -0.299735
  C      -0.594006     -0.541570      0.022144
  H      -0.050083      1.127108      1.282611
  H      -0.589698      1.595546     -0.338265
  C      -2.058792     -0.638815      0.448790
  H      -0.491955     -0.819239     -1.030418
  H      -0.012415     -1.248042      0.620654

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C	-3.003048	0.192099	-0.413844	
H	-2.362586	-1.685338	0.407733	
H	-2.149170	-0.335007	1.494731	
H	-2.888828	-0.063703	-1.468319	
H	-2.818082	1.260625	-0.308419	
H	-4.040996	0.013453	-0.136954	
Rotational constants (GHz):			6.3154700	1.1726500 1.0738000
Vibrational harmonic frequencies (cm-1):				
45.7360	106.3304			122.8886
148.0897	217.7402			280.4544
299.1437	364.9871			437.6733
532.2488	581.3161			753.6585
803.8979	903.9498			918.3607
974.5735	984.4548			1017.5488
1084.3550	1100.7672			1139.4980
1186.7538	1265.0300			1291.3404
1329.9892	1349.4611			1380.5677
1417.7881	1419.9657			1430.9399
1488.7497	1493.9153			1502.9165
1511.1389	1513.3398			3041.2364
3055.1677	3055.8566			3064.1792
3088.3174	3097.6450			3126.4008
3133.2739	3140.8159			3783.6673
Zero-point correction (Hartree): 0.145771				

C4H9O3H.pmmtt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92053146

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.291168	-1.154473	0.021886
O	-1.626173	-0.859310	-0.364230
O	-2.131815	0.113308	0.518686
O	-2.185865	1.323865	-0.181693
H	-1.298071	1.688205	-0.060272
C	0.672272	0.009101	-0.122880
H	-0.284508	-1.538896	1.045114
H	-0.015682	-1.967537	-0.652140
C	2.116033	-0.428605	0.099469
H	0.562646	0.445147	-1.119216
H	0.426169	0.780372	0.614258
C	3.094993	0.733882	0.003689
H	2.201650	-0.903556	1.079836
H	2.375524	-1.191787	-0.637908
H	2.870679	1.492850	0.754184
H	3.038273	1.208559	-0.976555
H	4.121360	0.404299	0.157610
Rotational constants (GHz):			5.3559200 1.1865700 1.0248400
Vibrational harmonic frequencies (cm-1):			
79.6046	96.4903		111.1701
157.7154	196.9296		251.7744
322.1560	359.3746		404.0869
524.2487	583.3267		753.0999
809.3282	915.9273		922.5280
963.4472	1001.9611		1033.4772
1082.2480	1094.3730		1145.6754
1205.6141	1267.9205		1284.4421
1327.5365	1335.6944		1383.8544
1414.8811	1419.9042		1429.2675
1488.0622	1494.4562		1503.7967
1504.8352	1516.5270		3032.4688
3052.4865	3058.4648		3061.1948
3075.0780	3092.8490		3116.4008
3127.9689	3138.7352		3784.9307
Zero-point correction (Hartree): 0.145635			

C4H9O3H.pmpmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91986580

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.115397	1.128514	0.651171
O	-1.149095	0.986693	-0.318692
O	-1.292547	-0.366691	-0.653630
O	-2.203805	-0.930058	0.255190
H	-1.626373	-1.346462	0.909607
C	1.281447	1.103790	0.057916

H	-0.319136	2.100926	1.100043
H	-0.249817	0.376565	1.433224
C	1.698431	-0.210297	-0.599697
H	1.353447	1.916015	-0.667448
H	1.978628	1.338803	0.868195
C	1.677340	-1.401228	0.350195
H	1.054259	-0.410964	-1.455965
H	2.708386	-0.083890	-0.993310
H	0.661104	-1.645800	0.661671
H	2.263430	-1.199058	1.248741
H	2.088719	-2.290356	-0.125213
Rotational constants (GHz): 3.6660800 1.8657200 1.4558800			
Vibrational harmonic frequencies (cm-1):			
67.9840	97.7071	141.6935	
154.9378	245.2972	262.2718	
341.9590	363.2220	427.9435	
555.4535	583.3399	747.0647	
824.8019	866.3201	908.9096	
952.8170	989.3271	1004.2408	
1051.4887	1113.8622	1137.5048	
1154.0792	1265.5945	1288.1673	
1332.2563	1369.2541	1396.7321	
1404.6777	1408.9555	1423.4472	
1472.9795	1488.9228	1493.4415	
1503.6512	1510.5559	3046.7528	
3056.3548	3063.6940	3071.8937	
3097.7411	3106.9136	3119.8265	
3126.8709	3135.2850	3786.8421	
Zero-point correction (Hartree): 0.145719			

C4H9O3H.pmpmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91701352

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.237200	-1.350604	-0.019989
O	0.907363	-0.420574	-0.867364
O	1.199100	0.742872	-0.141303
O	2.470676	0.570306	0.429656
H	2.266135	0.272356	1.325985
C	-1.261725	-1.140029	0.091102
H	0.453592	-2.318582	-0.473403
H	0.713063	-1.335037	0.965002
C	-1.703920	0.204471	0.677679
H	-1.708650	-1.272167	-0.897249
H	-1.634486	-1.958036	0.712873
C	-1.837557	1.307426	-0.368009
H	-2.669048	0.070556	1.168593
H	-1.002707	0.511489	1.457319
H	-2.599636	1.039383	-1.101254
H	-0.904958	1.472548	-0.903155
H	-2.134401	2.249082	0.092671
Rotational constants (GHz): 3.9210700 1.7273900 1.4158500			
Vibrational harmonic frequencies (cm-1):			
55.1088	102.7586	129.0109	
158.1073	206.2455	293.5325	
316.7854	346.8631	412.9223	
535.2419	580.8291	765.5544	
824.7875	874.6773	908.5072	
958.2331	986.8822	1005.1102	
1059.5570	1117.1460	1124.1111	
1177.2850	1264.8666	1294.2100	
1326.2634	1371.8581	1397.1715	
1398.8429	1416.5111	1420.2438	
1476.6893	1484.5953	1495.1067	
1504.3368	1510.3549	3049.7419	
3051.5567	3057.2664	3065.0384	
3093.2765	3094.1108	3114.8010	
3128.5851	3156.0770	3798.4933	
Zero-point correction (Hartree): 0.145596			

C4H9O3H.pmpmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91984032

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.562497	1.214629	0.486401
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O	-1.618004	0.795885	-0.370282
O	-1.473172	-0.559333	-0.695531
O	-1.823399	-1.319375	0.433095
H	-0.960366	-1.527287	0.820409
C	0.838807	0.976427	-0.053559
H	-0.766731	2.279900	0.589529
H	-0.691384	0.755423	1.471926
C	1.412530	-0.415760	0.204272
H	0.845679	1.195793	-1.123550
H	1.497369	1.708909	0.421673
C	2.886487	-0.503649	-0.171496
H	1.295126	-0.657060	1.266303
H	0.852907	-1.158596	-0.365937
H	3.477655	0.207628	0.406630
H	3.027464	-0.271840	-1.227744
H	3.286921	-1.500179	0.008793
Rotational constants (GHz):			
	4.2628400	1.5355000	1.2686800
Vibrational harmonic frequencies (cm-1):			
78.1998	90.3343		121.5697
193.4044	242.3679		262.6332
321.7203	381.9275		434.9429
546.9775	586.4964		751.2915
829.7388	880.8932		917.4149
963.2844	992.0595		1018.5567
1068.8235	1111.8732		1143.1000
1170.4404	1269.4509		1307.1015
1325.8389	1333.0727		1395.9992
1406.9459	1415.1057		1425.3898
1472.3989	1498.7177		1501.6653
1505.1079	1518.6190		3031.0586
3045.6439	3050.9384		3060.3062
3087.8003	3105.0896		3124.7339
3129.1178	3137.4032		3764.5636
Zero-point correction (Hartree): 0.145849			

C4H9O3H.pmpmm

E (RM062X/Aug-CC-pVTZ) (Hartree): -383.91930631

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.235780	1.198971	0.381485
O	0.777036	0.007304	0.941229
O	1.292011	-0.793946	-0.084988
O	2.583384	-0.323692	-0.384302
H	2.435563	0.216589	-1.171889
C	-0.888765	0.979539	-0.613860
H	-0.123980	1.732757	1.262548
H	1.046853	1.789240	-0.055934
C	-2.098008	0.223781	-0.061199
H	-1.195684	1.973743	-0.947403
H	-0.503342	0.462262	-1.495663
C	-1.911692	-1.289151	0.014181
H	-2.344649	0.617648	0.928575
H	-2.956923	0.440183	-0.698742
H	-1.130720	-1.564337	0.718881
H	-1.634107	-1.688375	-0.962642
H	-2.836355	-1.775881	0.323110
Rotational constants (GHz):			
	4.4976400	1.5965400	1.3848000
Vibrational harmonic frequencies (cm-1):			
46.1144	52.3266		95.1205
200.0773	229.6937		268.8168
347.8992	368.7804		434.2336
553.5095	583.4885		766.4103
833.2963	850.6476		913.9776
958.4578	972.3579		1005.0198
1061.4119	1117.4887		1122.3725
1188.8912	1263.2573		1290.9454
1321.2421	1374.9042		1395.2775
1404.2794	1413.5056		1418.0697
1476.9436	1489.4764		1498.6179
1503.7470	1516.3203		3043.9632
3049.3255	3058.7453		3064.7787
3089.5365	3092.9468		3112.7174
3127.1267	3159.7632		3797.8297
Zero-point correction (Hartree): 0.145652			

C4H9O3H.pmpmm

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E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92107065
Electronic state : 1-A
Cartesian coordinates (Angs):
  C      0.116959      0.353841      0.990260
  O      0.740927     -0.808012      0.454448
  O      1.525072     -0.447207     -0.647624
  O      2.745241      0.053579     -0.158703
  H      2.616712      1.010328     -0.208098
  C     -0.739105      1.100517     -0.018328
  H     -0.484456     -0.052095      1.803560
  H      0.876239      1.003233      1.434761
  C     -1.700646      0.198117     -0.787766
  H     -1.298551      1.860359      0.534282
  H     -0.097108      1.633224     -0.721674
  C     -2.625665     -0.607881      0.116657
  H     -2.293180      0.820412     -1.459863
  H     -1.123575     -0.480907     -1.416887
  H     -3.152814      0.042033      0.818235
  H     -2.069627     -1.347435      0.692734
  H     -3.372820     -1.143603     -0.466966
Rotational constants (GHz):      5.7280800      1.3537000      1.3352300
Vibrational harmonic frequencies (cm-1):
  44.7693      62.5210      118.1934
  205.6576      219.7573      292.0304
  357.2423      371.4844      436.7486
  571.8900      616.3836      734.8637
  829.3532      859.8777      915.5724
  952.9292      978.5582     1004.7658
 1049.6506     1109.7887     1137.3431
 1170.1745     1267.0215     1278.2117
 1322.9851     1369.1548     1391.4313
 1401.6705     1411.8215     1419.1552
 1481.1692     1494.4937     1501.1610
 1504.6196     1520.5352     3051.2354
 3055.2615     3061.8766     3070.4973
 3095.3359     3104.3757     3124.5078
 3127.3438     3137.3586     3796.0839
Zero-point correction (Hartree): 0.145864

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C4H9O3H.pmppt

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E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92119659
Electronic state : 1-A
Cartesian coordinates (Angs):
  C     -0.402071      1.142217      0.169273
  O     -1.112793      0.433422     -0.840909
  O     -1.558941     -0.787825     -0.323277
  O     -2.751267     -0.541874      0.382179
  H     -2.452490     -0.512599      1.300766
  C      0.826084      0.409274      0.673526
  H     -0.127241      2.068354     -0.337797
  H     -1.088499      1.398074      0.981415
  C      1.811793      0.057687     -0.433337
  H      1.310894      1.047883      1.417152
  H      0.521258     -0.500642      1.195568
  C      3.049020     -0.648368      0.104572
  H      1.311445     -0.573960     -1.168272
  H      2.102874      0.971682     -0.957720
  H      2.775819     -1.575667      0.609980
  H      3.575239     -0.020868      0.825485
  H      3.745754     -0.896904     -0.694727
Rotational constants (GHz):      5.8598600      1.1935700      1.1415300
Vibrational harmonic frequencies (cm-1):
  27.9580      75.0107      89.1036
 185.2680      237.0993      262.8771
 308.5519      368.2443      436.6571
 570.2076      593.1808      742.7356
 834.0584      861.6096      913.1483
 956.2450      976.2244     1010.4624
1064.9112     1105.6957     1142.6810
1188.5071     1267.1588     1287.3056
1331.6699     1341.8191     1397.8354
1409.7305     1412.4089     1414.3384
1479.2481     1496.1221     1498.4788
1504.8816     1512.0690     3047.0324
3053.6198     3056.8681     3060.6708

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3085.5985	3102.9720	3115.4001
3126.5068	3135.5985	3799.3576

Zero-point correction (Hartree): 0.145546

C4H9O3H.pmptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91980686

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.034311	0.530274	0.264160
O	-1.272644	0.951509	-0.294069
O	-2.078796	-0.169648	-0.523891
O	-2.768230	-0.444613	0.671190
H	-2.249138	-1.162230	1.057202
C	0.810893	-0.277635	-0.702181
H	0.444966	1.471263	0.533231
H	-0.219805	-0.020430	1.193402
C	2.100848	-0.786283	-0.062554
H	0.218815	-1.119313	-1.062837
H	1.042762	0.346598	-1.568004
C	3.027968	0.330016	0.408186
H	1.854663	-1.437732	0.780366
H	2.625655	-1.410057	-0.786986
H	2.590500	0.901254	1.227123
H	3.239348	1.024855	-0.406297
H	3.977200	-0.070425	0.761285

Rotational constants (GHz):	6.8558900	1.0783500	1.0549700
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Vibrational harmonic frequencies (cm-1):

46.4356	62.7580	110.2593
168.6717	232.0421	290.5644
292.2749	345.5601	430.6257
565.4064	577.4024	748.5016
799.8519	898.7291	913.9331
963.3058	972.8334	1005.7815
1080.8487	1098.5035	1138.5672
1185.5350	1265.8136	1290.9564
1326.8397	1345.5615	1378.4923
1404.1445	1415.7039	1422.7252
1488.3721	1494.4227	1504.5214
1509.5301	1513.6107	3032.6380
3050.5770	3060.3990	3066.5307
3095.1756	3108.6807	3126.5099
3130.5974	3136.7080	3800.7964

Zero-point correction (Hartree): 0.145570

C4H9O3H.pmptp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91958784

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.077364	-0.457274	0.667165
O	1.410757	-0.886645	0.418997
O	1.966592	-0.088927	-0.588338
O	2.489504	1.063974	0.025436
H	1.799083	1.721324	-0.132069
C	-0.856416	-0.715530	-0.499884
H	-0.217173	-1.042955	1.539929
H	0.090617	0.593933	0.967232
C	-2.311298	-0.388313	-0.169651
H	-0.531633	-0.125424	-1.359290
H	-0.762317	-1.765975	-0.779204
C	-2.556492	1.090519	0.115467
H	-2.934760	-0.699272	-1.008648
H	-2.632018	-0.985705	0.687751
H	-2.191027	1.707302	-0.707659
H	-2.055471	1.417700	1.026422
H	-3.619068	1.295446	0.238198

Rotational constants (GHz):	5.1910600	1.2297900	1.1081800
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Vibrational harmonic frequencies (cm-1):

38.6052	53.4435	114.4169
156.1123	236.4551	287.7373
301.5770	346.8188	416.2202
568.0562	577.6878	751.2099
800.8967	898.6439	910.7370
959.0284	979.5565	1002.1018
1076.6380	1100.6101	1136.5187
1190.3507	1265.9477	1289.8882

1327.5771	1346.2627	1377.4260
1402.8970	1414.6519	1422.1745
1489.8908	1494.4948	1504.8949
1509.0486	1514.0743	3052.8058
3055.8265	3060.7962	3067.0383
3095.2809	3099.0458	3120.6668
3126.3493	3136.6589	3801.4728

Zero-point correction (Hartree): 0.145526

C4H9O3H.pmpptt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92061744

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.291524	0.779692	0.412859
O	-1.476605	0.894316	-0.364054
O	-1.973836	-0.387023	-0.630743
O	-2.787752	-0.757692	0.455000
H	-2.202818	-1.321158	0.978283
C	0.862218	0.142908	-0.335076
H	-0.065204	1.813354	0.678770
H	-0.514857	0.245253	1.342336
C	2.125745	0.094227	0.515997
H	0.582980	-0.866842	-0.642186
H	1.046306	0.713964	-1.247655
C	3.296759	-0.537087	-0.225612
H	2.391674	1.107184	0.828883
H	1.925378	-0.467558	1.432160
H	3.530110	0.025915	-1.129886
H	3.059980	-1.558971	-0.524047
H	4.192816	-0.566385	0.392712

Rotational constants (GHz): 6.7632700 1.0132800 0.9788900

Vibrational harmonic frequencies (cm-1):

52.5297	69.4918	107.4474
146.9197	210.2375	248.9574
319.1229	361.6854	404.8093
557.7020	576.3922	737.9204
803.9515	911.2166	922.2892
952.3718	985.7696	1033.2334
1081.7019	1091.4715	1145.8802
1202.4614	1266.8188	1286.6767
1326.6393	1329.5102	1382.8966
1405.1056	1414.9205	1420.4646
1492.5148	1492.9564	1503.7514
1504.7825	1516.4776	3039.1883
3045.6357	3060.6313	3065.8129
3074.2353	3100.0949	3119.3068
3128.5908	3137.0400	3802.1620

Zero-point correction (Hartree): 0.145438

C4H9O3H.pmtmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92093799

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.142174	0.538272	0.562786
O	-0.757192	-0.128391	-0.532787
O	-1.881611	-0.818531	-0.072025
O	-2.956338	0.089016	-0.040128
H	-2.987792	0.347373	0.890440
C	1.139255	1.158343	0.039535
H	-0.811848	1.315689	0.940360
H	0.052853	-0.186989	1.355710
C	2.107611	0.150983	-0.579563
H	0.883708	1.925900	-0.692309
H	1.618192	1.664057	0.881739
C	2.489966	-0.981502	0.365941
H	1.662923	-0.264119	-1.484196
H	3.004920	0.688703	-0.889313
H	1.637787	-1.627865	0.576026
H	2.860956	-0.592244	1.316305
H	3.271473	-1.603822	-0.067431

Rotational constants (GHz): 6.2453500 1.2070100 1.1186200

Vibrational harmonic frequencies (cm-1):

50.9154	59.4177	121.4427
170.5186	233.3649	298.9369
317.5099	374.3082	418.4538

508.4033	613.5040	746.4092
842.9873	862.9056	942.8552
981.6786	1001.0082	1009.4141
1049.2322	1114.5609	1149.9184
1175.5886	1250.8983	1279.6585
1323.8420	1373.4676	1392.3917
1404.4074	1414.0831	1421.6915
1478.0410	1495.6630	1504.3351
1510.2011	1532.7626	3045.5982
3055.9418	3061.5658	3072.8611
3090.6627	3103.5781	3113.3606
3128.6944	3136.8111	3801.3338

Zero-point correction (Hartree): 0.145883

C4H9O3H.pmtmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91941430

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.164233	0.795482	0.336017
O	-0.696088	-0.344615	-0.332223
O	-1.878016	-0.731726	0.305736
O	-2.924870	0.042574	-0.228527
H	-3.038069	0.733988	0.436836
C	1.173367	1.121379	-0.306422
H	-0.859633	1.630239	0.214545
H	-0.052876	0.566190	1.399750
C	2.343578	0.276956	0.193198
H	1.062756	1.014990	-1.388310
H	1.382275	2.175076	-0.114519
C	2.196827	-1.217651	-0.068050
H	3.254404	0.641269	-0.285436
H	2.470803	0.451066	1.264923
H	2.018476	-1.410267	-1.126596
H	1.357078	-1.638242	0.482333
H	3.099336	-1.751178	0.228135

Rotational constants (GHz): 6.0193500 1.2608700 1.1087400

Vibrational harmonic frequencies (cm-1):

38.9787	78.9293	94.0930
150.0311	248.6559	277.3020
321.2514	349.6940	407.5700
493.9174	607.0076	778.8161
820.2140	872.1026	940.1645
983.6275	995.2992	1009.4939
1050.8000	1115.8317	1144.9034
1181.1387	1253.9023	1292.5735
1313.6668	1379.2001	1390.8575
1403.7731	1417.9417	1424.3767
1475.7152	1490.8652	1502.9649
1508.1061	1520.9489	3037.3692
3050.6132	3060.9396	3065.8650
3084.4733	3090.7829	3107.2662
3132.0486	3146.5871	3799.2766

Zero-point correction (Hartree): 0.145598

C4H9O3H.pmtmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92132482

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.335652	0.658989	0.399097
O	-0.917629	-0.461533	-0.257049
O	-2.187187	-0.693468	0.277779
O	-3.093080	0.150811	-0.391081
H	-3.195538	0.884743	0.228972
C	1.084330	0.780636	-0.114797
H	-0.911290	1.557304	0.159942
H	-0.354717	0.487466	1.478660
C	1.971051	-0.397156	0.272740
H	1.056933	0.886282	-1.201833
H	1.504743	1.707713	0.282605
C	3.394835	-0.230138	-0.240551
H	1.977462	-0.495063	1.361378
H	1.537695	-1.317346	-0.119827
H	3.850733	0.676652	0.159967
H	3.407372	-0.154269	-1.328610
H	4.022388	-1.073945	0.042608

Rotational constants (GHz): 9.5232000 0.9686300 0.9305600
 Vibrational harmonic frequencies (cm-1):
 52.2357 78.6777 90.5278
 152.5100 241.0773 260.4764
 303.8048 326.6120 404.5393
 513.9300 621.7399 739.8170
 846.2442 866.4491 941.7509
 985.4516 988.7275 1030.3933
 1061.6777 1103.2969 1161.0686
 1187.6253 1255.0470 1285.3945
 1330.7851 1340.2036 1400.7993
 1411.0755 1414.9411 1416.9055
 1478.4189 1497.0665 1503.9336
 1512.2918 1521.5143 3039.1240
 3053.8981 3057.4593 3061.9599
 3085.3408 3094.8375 3109.3032
 3128.7139 3135.8932 3802.7416
 Zero-point correction (Hartree): 0.145566

C4H9O3H.pmtpm

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.91987666
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.094786 -1.033846 0.335893
 O -0.758291 -0.301566 -0.690394
 O -2.114963 -0.206314 -0.371621
 O -2.274656 0.916053 0.463825
 H -2.318842 0.520077 1.344067
 C 1.376536 -1.103161 -0.036735
 H -0.220463 -0.514881 1.292511
 H -0.544771 -2.026084 0.400863
 C 2.184511 0.132863 0.353183
 H 1.801246 -1.982256 0.450369
 H 1.443293 -1.277154 -1.113441
 C 1.689725 1.428465 -0.279970
 H 2.172816 0.230096 1.442172
 H 3.225893 -0.036188 0.073449
 H 0.683097 1.677250 0.053227
 H 1.656192 1.340124 -1.366460
 H 2.348903 2.257706 -0.025461
 Rotational constants (GHz): 4.4393800 1.4942300 1.2635500
 Vibrational harmonic frequencies (cm-1):
 47.9827 80.4942 118.4742
 158.8357 261.1890 278.3865
 319.9956 353.0917 411.1833
 479.6182 610.7974 780.4107
 822.7256 869.0021 941.7087
 977.3662 995.9139 1016.5694
 1048.3376 1114.9072 1146.3949
 1178.7259 1253.8700 1291.7280
 1313.4762 1376.8049 1387.4251
 1402.4990 1419.1346 1425.7202
 1476.4321 1491.5659 1503.2000
 1509.5188 1519.7025 3031.4003
 3049.9306 3061.8750 3064.9261
 3088.2608 3095.0390 3107.6002
 3132.3475 3143.3604 3802.5540
 Zero-point correction (Hartree): 0.145713

C4H9O3H.pmtpp

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92134709
 Electronic state : 1-A
 Cartesian coordinates (Angs):
 C -0.090772 -0.847078 0.622938
 O -0.793196 -0.552949 -0.578160
 O -2.130969 -0.292900 -0.268683
 O -2.225385 1.066456 0.084510
 H -2.236170 1.033763 1.050165
 C 1.354089 -1.100309 0.238199
 H -0.160888 0.008474 1.300526
 H -0.539089 -1.720995 1.099224
 C 1.995243 0.054015 -0.533317
 H 1.905255 -1.279946 1.164585
 H 1.408790 -2.016762 -0.350883
 C 1.864028 1.399095 0.171284

H	3.049198	-0.182308	-0.686428	
H	1.540821	0.119368	-1.521884	
H	2.224503	1.342269	1.200724	
H	0.825634	1.731673	0.190325	
H	2.442814	2.165275	-0.342315	
Rotational constants (GHz):				4.3560300 1.5197600 1.2713600
Vibrational harmonic frequencies (cm-1):				
47.3448	71.9374			143.3128
169.7206	239.7107			300.3611
334.1412	373.6047			427.5013
498.8338	624.8309			743.6226
840.5070	861.3410			942.1675
982.2997	992.8822			1016.0772
1047.7681	1114.1986			1152.6667
1174.7806	1253.7800			1280.2872
1323.3845	1372.9329			1388.6328
1402.3004	1413.2964			1425.1827
1479.0821	1494.4714			1503.2141
1510.3158	1531.2532			3046.7498
3053.9047	3060.7625			3073.9108
3093.7524	3104.2768			3113.2226
3127.9399	3135.8597			3802.3086
Zero-point correction (Hartree): 0.146009				

C4H9O3H.pmtpt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92130931

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.339322	0.826374	0.449785	
O	0.965769	0.187222	-0.656420	
O	2.348728	0.188262	-0.456177	
O	2.668500	-0.947050	0.310857	
H	2.740140	-0.586311	1.204354	
C	-1.147810	0.845099	0.161559	
H	0.541290	0.254380	1.361477	
H	0.744919	1.834504	0.553998	
C	-1.773693	-0.544308	0.116485	
H	-1.630829	1.443912	0.937601	
H	-1.314542	1.361416	-0.786712	
C	-3.270129	-0.485511	-0.158546	
H	-1.275091	-1.138421	-0.649679	
H	-1.590522	-1.048226	1.069058	
H	-3.468487	-0.007296	-1.118601	
H	-3.786840	0.090013	0.611119	
H	-3.710149	-1.481372	-0.184402	
Rotational constants (GHz): 6.8096000 1.0537700 0.9959900				
Vibrational harmonic frequencies (cm-1):				
47.0712	70.6329			107.7731
146.2844	247.1244			263.1565
299.3310	324.4167			399.2624
498.9849	629.5386			736.8468
842.4106	864.5515			942.2829
977.7870	991.9590			1033.6506
1060.8749	1104.1627			1163.1143
1183.8257	1254.8339			1286.0705
1328.1163	1338.4633			1399.4180
1406.9957	1414.9785			1418.8216
1478.4079	1497.1315			1505.3972
1512.6105	1518.9771			3032.6542
3051.9044	3056.8969			3060.2716
3089.6188	3095.6966			3108.2373
3128.0320	3135.8608			3803.4460
Zero-point correction (Hartree): 0.145479				

C4H9O3H.pmttm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92019635

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.072861	-0.159394	0.282767
O	-1.246936	-0.797392	-0.201758
O	-2.362340	-0.224387	0.416279
O	-2.723087	0.915020	-0.326457
H	-2.331078	1.634567	0.185486
C	1.101362	-0.852981	-0.378523
H	-0.101564	0.900329	0.015879

H	-0.029715	-0.258549	1.371293	
C	2.444418	-0.382216	0.174734	
H	0.992268	-1.927500	-0.225415	
H	1.056019	-0.674480	-1.454727	
C	2.699630	1.107942	-0.026151	
H	2.501584	-0.624771	1.238577	
H	3.235066	-0.953139	-0.313355	
H	2.011458	1.717621	0.559620	
H	2.578807	1.383383	-1.075228	
H	3.710763	1.376503	0.276400	
Rotational constants (GHz):				6.2227200 1.0766400 0.9725300
Vibrational harmonic frequencies (cm-1):				
51.2782	72.2956	113.0437		
150.4113	190.4090	274.2600		
305.5690	348.7005	426.0618		
484.6040	599.7880	759.8297		
818.4814	895.5335	940.9950		
971.9192	1006.6721	1012.4361		
1077.5012	1103.1558	1162.6987		
1187.1084	1248.3521	1296.3337		
1317.3895	1353.7320	1379.7917		
1403.2306	1416.9711	1429.1109		
1492.7519	1496.6725	1508.6580		
1512.9540	1525.1386	3039.6530		
3057.3042	3061.1888	3067.8743		
3083.7565	3097.2137	3118.1363		
3128.2221	3136.0868	3802.3356		
Zero-point correction (Hartree): 0.145633				

C4H9O3H.pmttp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92026385

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.072688	-0.056196	-0.047865	
O	-1.223974	0.717295	-0.359085	
O	-2.298067	-0.143668	-0.601761	
O	-2.875629	-0.465573	0.640408	
H	-2.490806	-1.330226	0.835141	
C	1.086833	0.914512	0.055430	
H	-0.221186	-0.570296	0.908323	
H	0.080467	-0.794507	-0.837116	
C	2.363406	0.246748	0.561070	
H	1.260523	1.360562	-0.925923	
H	0.796741	1.721562	0.729498	
C	2.863095	-0.876241	-0.341724	
H	3.137268	1.009822	0.651508	
H	2.193533	-0.139541	1.569069	
H	2.978606	-0.524893	-1.368417	
H	2.173292	-1.720254	-0.355366	
H	3.829052	-1.249602	-0.004675	
Rotational constants (GHz):				
6.8595400 1.0136700 0.9795900				
Vibrational harmonic frequencies (cm-1):				
49.4260	80.0769	121.0881		
140.5751	192.6168	277.1529		
310.4913	353.0967	425.6997		
487.9273	601.1044	759.3951		
821.0289	895.2644	941.4363		
973.8179	1007.8529	1010.7658		
1078.3228	1103.6818	1163.0454		
1185.9311	1249.8157	1296.2549		
1318.6674	1353.9127	1380.4694		
1404.1391	1417.6754	1428.3324		
1492.8720	1496.7712	1508.9197		
1513.0738	1525.8752	3028.1393		
3056.6305	3060.9742	3067.5768		
3089.8860	3097.0645	3118.4959		
3128.7307	3135.7838	3800.2321		
Zero-point correction (Hartree): 0.145689				

C4H9O3H.pmttt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92108675

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.262527	0.132990	0.332826
O	-1.262849	-0.756494	-0.144129

O	-2.500210	-0.369945	0.379090
O	-3.025792	0.628471	-0.461720
H	-2.803911	1.441624	0.010665
C	1.068132	-0.384435	-0.170313
H	-0.450126	1.138919	-0.056292
H	-0.293035	0.156412	1.425111
C	2.223742	0.504660	0.274369
H	1.215561	-1.401282	0.199055
H	1.038304	-0.440847	-1.260282
C	3.567175	-0.012138	-0.223133
H	2.061392	1.520876	-0.093095
H	2.234180	0.567186	1.365208
H	3.584681	-0.058244	-1.312529
H	3.758928	-1.017110	0.154327
H	4.385698	0.629742	0.099405
Rotational constants (GHz): 10.3387200 0.8718300 0.8485300			
Vibrational harmonic frequencies (cm-1):			
58.6870	74.7703		129.7154
135.2249	163.5078		249.4457
310.0367	358.6511		390.3216
490.3129	608.8459		742.4133
822.3600	914.1039		942.8470
962.1860	1010.5549		1053.5372
1084.8999	1092.5941		1167.9786
1194.8828	1251.8711		1298.1991
1316.2160	1329.9918		1388.2639
1405.9812	1416.6971		1427.6727
1493.3682	1500.2751		1504.2154
1512.8864	1526.9188		3034.2786
3050.1223	3061.0886		3067.4993
3078.4080	3082.2785		3114.9454
3129.9278	3136.9912		3800.4960
Zero-point correction (Hartree): 0.145544			

C4H9O3H.ppmmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92394572

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.037098	1.246884	0.234585
O	0.929363	0.715058	-0.745489
O	2.042923	0.178509	-0.083181
O	1.830114	-1.202223	0.062695
H	2.128495	-1.545871	-0.790421
C	-0.679357	0.190181	1.054021
H	0.595404	1.931999	0.874397
H	-0.661173	1.830536	-0.366398
C	-1.479020	-0.811141	0.224506
H	0.050352	-0.336344	1.669810
H	-1.349072	0.720968	1.737373
C	-2.542480	-0.164166	-0.656150
H	-0.790257	-1.388029	-0.392678
H	-1.952907	-1.518662	0.906612
H	-2.095786	0.430449	-1.453137
H	-3.190650	0.491813	-0.071369
H	-3.171047	-0.918164	-1.128158
Rotational constants (GHz): 4.3781600 1.5821000 1.4274400			
Vibrational harmonic frequencies (cm-1):			
53.7805	89.2316		131.9488
177.1547	224.9437		282.8455
360.2447	392.8784		466.6670
504.5186	625.4272		732.2938
830.2670	854.0718		918.1112
962.9806	974.1472		1009.9993
1046.3842	1106.9499		1138.6886
1168.0647	1264.5263		1286.9159
1329.9279	1368.0125		1395.5363
1410.2536	1419.5625		1422.3472
1477.8172	1487.7584		1495.4219
1504.6146	1518.0286		3051.4033
3055.4603	3072.3663		3076.2311
3106.7655	3108.8109		3127.4300
3129.3940	3135.0274		3791.8155
Zero-point correction (Hartree): 0.146001			

C4H9O3H.ppmmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92208615
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.107357	1.385574	0.255563
O	-0.969583	0.430393	0.877703
O	-1.947588	0.046140	-0.051097
O	-1.549639	-1.180238	-0.607177
H	-1.837180	-1.813320	0.065034
C	0.843458	0.816622	-0.783273
H	-0.732749	2.171338	-0.170951
H	0.442269	1.802811	1.102787
C	2.024476	0.034772	-0.211502
H	0.277037	0.200366	-1.483240
H	1.225770	1.666358	-1.354130
C	1.645027	-1.257084	0.504460
H	2.709655	-0.198351	-1.028662
H	2.577447	0.684119	0.473359
H	1.081592	-1.910780	-0.161696
H	1.020963	-1.062136	1.375165
H	2.536051	-1.790061	0.835410

Rotational constants (GHz): 3.6820400 1.8628600 1.5296600
 Vibrational harmonic frequencies (cm-1):

39.9941	96.5586	120.1401
169.2454	258.0491	294.6101
330.5658	360.1210	464.6194
477.8807	598.5840	781.5351
814.8887	859.1519	917.4538
958.6134	970.3196	1008.2757
1052.4669	1117.5614	1122.2377
1186.8109	1259.6845	1303.9983
1329.4859	1379.6882	1396.5538
1414.7649	1419.4554	1424.1239
1476.7731	1480.0709	1495.0650
1501.4973	1511.8972	3044.3126
3059.0454	3065.3024	3066.0501
3085.3556	3107.6378	3117.2439
3132.4151	3145.3350	3789.7061

Zero-point correction (Hartree): 0.145814

C4H9O3H.ppmmt

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92468447
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	-0.540570	-1.407656	0.106913
O	-1.429928	-0.570383	-0.634253
O	-2.001135	0.356984	0.248324
O	-1.261684	1.547911	0.148610
H	-1.663054	1.972876	-0.621614
C	0.698437	-0.693759	0.608532
H	-1.099179	-1.865399	0.924988
H	-0.283323	-2.182152	-0.618494
C	1.562468	-0.121253	-0.507148
H	0.400473	0.100853	1.294919
H	1.277008	-1.413859	1.194298
C	2.757677	0.650269	0.035506
H	1.905034	-0.935337	-1.151661
H	0.949928	0.533945	-1.127116
H	3.384434	0.012227	0.660597
H	2.424440	1.489421	0.647591
H	3.378150	1.045726	-0.767773

Rotational constants (GHz): 4.0971100 1.6055200 1.2968200
 Vibrational harmonic frequencies (cm-1):

56.1927	106.3263	127.3681
186.4162	239.9772	262.0869
315.5377	374.5316	460.2023
501.3033	625.4994	742.0224
837.7188	858.2670	916.2580
962.1487	979.1745	1011.0888
1065.0367	1103.5435	1146.1371
1187.7533	1267.7819	1294.6908
1331.5408	1345.4367	1407.1807
1412.0072	1413.5551	1421.7635
1481.0977	1485.5471	1496.6634
1504.6796	1511.7384	3050.2126
3053.9690	3056.0114	3067.0022
3095.3414	3106.0862	3118.0258

3126.6570 3131.9677 3790.5745
 Zero-point correction (Hartree): 0.145880

C4H9O3H.ppmpp

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92092946

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.104548	1.375450	-0.168623
O	-1.441648	0.883361	-0.242568
O	-1.423449	-0.445231	-0.694830
O	-1.617574	-1.265078	0.427859
H	-2.577680	-1.234647	0.539039
C	0.773886	0.731893	0.892382
H	0.345809	1.319807	-1.161327
H	-0.271141	2.427003	0.067351
C	1.431835	-0.600600	0.526574
H	1.567843	1.452999	1.109725
H	0.185331	0.625206	1.805216
C	2.288582	-0.531425	-0.732805
H	2.059225	-0.897826	1.369128
H	0.677852	-1.376850	0.416227
H	3.002072	0.293772	-0.680952
H	1.679390	-0.393235	-1.625748
H	2.854136	-1.452556	-0.867516

Rotational constants (GHz): 3.6558700 1.8107300 1.5280800

Vibrational harmonic frequencies (cm-1):

21.9964	82.9756	152.0235
167.1045	263.6258	286.0449
329.8898	387.5567	423.8018
502.6237	588.9800	744.0996
820.0489	867.3795	914.1741
962.3558	991.0195	1008.0937
1053.5384	1123.4527	1142.6728
1148.2413	1267.3832	1292.4058
1338.6842	1370.3878	1394.1533
1412.1695	1423.2263	1424.9032
1467.2839	1485.6837	1497.6639
1507.5690	1518.7308	3044.7849
3055.4103	3068.9943	3075.7922
3102.1403	3116.9122	3123.2031
3135.0802	3145.1802	3792.8902

Zero-point correction (Hartree): 0.145899

C4H9O3H.ppmpt

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92209269

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.610922	1.424482	0.076055
O	1.752329	0.607605	-0.182112
O	1.649942	-0.585056	0.546764
O	1.124199	-1.560941	-0.317624
H	1.908370	-1.838237	-0.810830
C	-0.707254	0.879061	-0.453088
H	0.556820	1.622286	1.149734
H	0.884586	2.349734	-0.431662
C	-1.462648	-0.023851	0.517560
H	-1.344528	1.733873	-0.696918
H	-0.514811	0.352977	-1.390317
C	-2.759905	-0.541580	-0.088566
H	-0.834310	-0.862209	0.812856
H	-1.679367	0.542762	1.427062
H	-2.555391	-1.141360	-0.976511
H	-3.409856	0.282731	-0.387377
H	-3.309955	-1.164101	0.615967

Rotational constants (GHz): 3.9602500 1.6800400 1.3117800

Vibrational harmonic frequencies (cm-1):

56.4029	106.7236	146.1648
175.3164	243.9902	261.7925
321.7040	366.8701	424.5836
496.7725	607.4946	733.0422
819.3846	882.5740	914.5251
965.8015	999.4256	1014.5255
1065.3884	1105.0538	1144.9911
1169.2441	1265.1572	1312.0204
1334.1800	1343.4018	1401.4849

1411.9625	1417.8941	1423.3289
1471.9627	1484.8004	1495.3331
1503.4957	1510.6414	3048.6864
3053.8673	3056.0455	3058.9506
3099.3816	3113.4628	3120.4545
3132.9987	3142.7432	3793.3042

Zero-point correction (Hartree): 0.145842

C4H9O3H.ppmtm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92271524

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.010585	0.905764	-0.203758
O	1.405301	0.955428	-0.370199
O	1.999588	0.198994	0.649357
O	2.241008	-1.086834	0.137432
H	3.074152	-0.964132	-0.337649
C	-0.616888	-0.451468	-0.506086
H	-0.249736	1.244202	0.805472
H	-0.365987	1.655843	-0.914087
C	-2.143094	-0.399287	-0.549241
H	-0.225008	-0.796772	-1.463915
H	-0.291592	-1.168914	0.248890
C	-2.779695	-0.006054	0.780713
H	-2.460754	0.298487	-1.328713
H	-2.513551	-1.380702	-0.847950
H	-2.545314	1.022632	1.054130
H	-2.423226	-0.652458	1.584364
H	-3.864584	-0.092618	0.736977

Rotational constants (GHz): 5.4156700 1.2296400 1.1590000

Vibrational harmonic frequencies (cm-1):

51.0414	97.4257	124.3793
132.8449	225.1600	285.6875
316.1500	366.0831	428.6703
511.7559	611.1741	755.3274
807.2830	898.2400	912.7033
958.7264	983.7300	1003.7927
1073.9700	1101.9040	1137.0683
1191.9813	1270.6238	1289.9341
1331.5874	1353.1158	1377.7565
1416.9684	1423.1859	1425.7677
1482.4828	1494.4623	1499.5222
1507.4798	1513.6933	3051.4934
3060.0016	3063.9522	3072.8673
3094.2774	3103.4508	3126.7488
3128.5752	3136.0548	3793.8288

Zero-point correction (Hartree): 0.145787

C4H9O3H.ppmtp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92285959

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.038836	0.826642	0.190629
O	1.293710	1.017532	-0.279230
O	2.154991	0.203600	0.470492
O	2.379086	-0.968280	-0.270373
H	3.073948	-0.692491	-0.883545
C	-0.600752	-0.553892	-0.087129
H	-0.072913	1.055340	1.259380
H	-0.589064	1.600384	-0.345673
C	-2.042350	-0.690031	0.400500
H	-0.545280	-0.750886	-1.160246
H	0.026144	-1.294908	0.407400
C	-3.024672	0.231325	-0.316231
H	-2.355869	-1.725505	0.263089
H	-2.079137	-0.500690	1.476544
H	-2.957747	0.100204	-1.397604
H	-2.832344	1.281415	-0.096329
H	-4.050364	0.020053	-0.016738

Rotational constants (GHz): 6.3422000 1.1868800 1.0758800

Vibrational harmonic frequencies (cm-1):

45.2776	106.7500	122.7682
137.2412	220.2204	285.7275
300.7009	362.1327	438.5134
506.6127	610.8090	748.8349

799.5792	902.2176	916.3995
964.1265	977.4463	1009.9123
1079.5915	1099.4679	1139.9873
1183.2525	1267.9276	1295.7075
1334.8811	1351.9440	1378.0243
1415.3947	1424.1972	1427.3354
1483.5491	1493.7567	1499.9625
1506.3547	1513.8401	3053.3225
3054.0499	3060.9328	3069.4997
3095.6720	3112.3037	3128.5720
3132.3685	3137.1067	3795.3467

Zero-point correction (Hartree): 0.145779

C4H9O3H.ppmTT

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92382446

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.284250	-1.138505	0.018091
O	-1.622390	-0.851724	-0.380282
O	-2.161537	0.087120	0.510645
O	-2.000094	1.357553	-0.066153
H	-2.754656	1.405235	-0.668872
C	0.683657	0.012386	-0.167009
H	-0.292820	-1.484035	1.054706
H	-0.016162	-1.980536	-0.623145
C	2.111677	-0.417661	0.149475
H	0.616948	0.374553	-1.195279
H	0.393742	0.840487	0.481139
C	3.106002	0.724673	-0.011708
H	2.156232	-0.801382	1.172051
H	2.395402	-1.247139	-0.503639
H	2.854505	1.551843	0.652898
H	3.094241	1.105951	-1.033424
H	4.122216	0.406070	0.216785

Rotational constants (GHz): 5.3660600 1.1950200 1.0330600

Vibrational harmonic frequencies (cm-1):

72.6675	99.4798	115.1666
138.2449	197.4509	251.6962
329.5552	374.1150	412.9032
496.1378	611.8130	742.7027
806.6366	913.5969	923.7654
953.5193	991.0790	1031.6943
1081.1570	1092.1961	1146.6000
1203.0043	1269.6403	1289.2933
1330.9197	1334.7693	1386.3036
1413.8287	1422.1656	1426.7652
1483.7801	1492.0905	1501.5603
1504.2239	1515.2390	3045.1651
3057.1547	3060.5666	3069.4259
3076.2124	3101.1790	3123.2711
3129.9567	3135.5599	3793.5576

Zero-point correction (Hartree): 0.145684

C4H9O3H.pppmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92423564

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.114201	1.122433	0.647409
O	-1.148540	0.975928	-0.328136
O	-1.279053	-0.382018	-0.654405
O	-2.050992	-0.979670	0.355160
H	-2.949997	-0.722448	0.107535
C	1.281295	1.105275	0.052549
H	-0.325042	2.094475	1.094050
H	-0.255607	0.360422	1.415121
C	1.707289	-0.212192	-0.593267
H	1.352968	1.914984	-0.676159
H	1.974160	1.347174	0.864540
C	1.668081	-1.397745	0.363398
H	1.074173	-0.416178	-1.457235
H	2.721962	-0.086065	-0.975359
H	0.647539	-1.631929	0.665454
H	2.249649	-1.191538	1.264385
H	2.084092	-2.289443	-0.103822

Rotational constants (GHz): 3.6665600 1.8969400 1.4767600

Vibrational harmonic frequencies (cm-1):

56.2723	95.7666	158.8444
171.8558	264.2851	267.0154
355.9694	383.6806	429.8078
560.5339	599.2248	751.2319
825.8522	866.6262	908.4330
953.4162	995.1110	1001.4664
1047.8769	1110.7484	1141.1247
1157.2031	1266.7105	1290.7080
1333.6479	1371.5448	1396.0098
1411.6886	1418.5441	1421.8802
1473.2770	1490.5822	1496.2555
1505.3545	1519.7477	3045.6147
3056.0999	3068.2698	3082.4519
3094.1318	3106.8021	3126.4122
3129.1093	3137.8800	3788.1007

Zero-point correction (Hartree): 0.146106

C4H9O3H.pppmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92119881
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.247460	-1.342221	-0.016268
O	0.910840	-0.399010	-0.862482
O	1.193909	0.756997	-0.119272
O	2.377459	0.508880	0.593747
H	3.056160	0.635039	-0.083871
C	-1.253744	-1.145731	0.082120
H	0.476747	-2.305634	-0.473176
H	0.726550	-1.307475	0.963733
C	-1.711428	0.192197	0.672437
H	-1.695902	-1.279965	-0.908363
H	-1.621398	-1.968615	0.700510
C	-1.852352	1.297233	-0.370079
H	-2.677790	0.047346	1.157958
H	-1.014908	0.502236	1.454028
H	-2.606914	1.024456	-1.109568
H	-0.918300	1.474688	-0.898870
H	-2.161519	2.234112	0.092409

Rotational constants (GHz): 3.9396500 1.7359000 1.4291300

Vibrational harmonic frequencies (cm-1):

70.3833	109.9083	140.1578
162.2877	209.8597	295.2182
335.9981	375.7999	406.6078
536.9069	602.2785	765.6070
824.2645	875.4614	907.0228
958.8917	989.4417	1003.5887
1055.1668	1116.1722	1121.7362
1179.9401	1267.0077	1295.0015
1330.1645	1372.2870	1398.9804
1412.2139	1417.3791	1421.8950
1477.8416	1487.2899	1495.9035
1503.9645	1509.8919	3049.7827
3061.4805	3063.6023	3074.3190
3092.4194	3097.1263	3125.1871
3127.5145	3154.7025	3787.4221

Zero-point correction (Hartree): 0.145953

C4H9O3H.pppmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92376626
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.404037	1.187691	0.336238
O	-1.241585	0.636575	-0.683244
O	-1.460436	-0.720937	-0.408320
O	-2.510111	-0.788123	0.522091
H	-3.288679	-0.655023	-0.036246
C	1.071623	0.951230	0.085363
H	-0.635180	2.253096	0.313671
H	-0.729571	0.786367	1.297709
C	1.498471	-0.511744	0.105985
H	1.341444	1.399344	-0.874359
H	1.624145	1.501095	0.853786
C	3.007017	-0.660534	-0.043074
H	1.165688	-0.972899	1.039107

H	0.992430	-1.048729	-0.696633	
H	3.531747	-0.159082	0.771578	
H	3.349431	-0.216616	-0.979083	
H	3.307154	-1.707536	-0.040826	
Rotational constants (GHz):		5.1143300	1.3099400	1.1493900
Vibrational harmonic frequencies (cm-1):				
59.7905		92.1235		124.6325
146.8711		238.1947		253.3822
313.2949		375.6079		417.9094
555.8897		601.6471		748.4216
834.2549		862.8987		914.0593
960.9644		983.4896		1011.7238
1059.5433		1099.5121		1142.3357
1182.2953		1270.1462		1299.3702
1333.1215		1346.0619		1406.7810
1413.3769		1414.1479		1421.4352
1475.5123		1488.1997		1494.0222
1504.0818		1510.5428		3042.6598
3056.2114		3060.6635		3072.4129
3084.3592		3104.9803		3124.4182
3127.5753		3135.1904		3788.6076
Zero-point correction (Hartree):		0.145695		

C4H9O3H.ppppm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92316948

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.221345	1.192362	0.357743
O	0.777721	-0.011940	0.886786
O	1.319447	-0.757399	-0.169374
O	2.581242	-0.212246	-0.459054
H	3.136353	-0.603396	0.229592
C	-0.931375	0.977451	-0.603951
H	-0.111452	1.714660	1.256499
H	1.023237	1.770397	-0.105502
C	-2.124762	0.217231	-0.023663
H	-1.248043	1.973814	-0.921615
H	-0.564617	0.469419	-1.497943
C	-1.938328	-1.296938	0.025334
H	-2.341807	0.597498	0.978483
H	-3.002909	0.441692	-0.631618
H	-1.133771	-1.581180	0.699440
H	-1.693548	-1.682292	-0.965684
H	-2.852000	-1.788573	0.358712
Rotational constants (GHz):		4.6408100	1.5617000
Vibrational harmonic frequencies (cm-1):			
32.3931		59.7437	103.6856
199.2002		227.0346	265.4313
357.9407		367.2343	429.8865
551.4366		597.3756	765.5836
834.3695		850.6335	913.1680
960.2096		974.1585	1004.3505
1056.6924		1117.5275	1117.9174
1189.3292		1264.0184	1294.1518
1324.3393		1375.2112	1398.8438
1410.4330		1416.3148	1421.8758
1478.9925		1486.0602	1495.3761
1502.5923		1515.0087	3048.1138
3059.8908		3064.2797	3069.4914
3088.7299		3101.2832	3119.6671
3126.3002		3157.3283	3791.1938
Zero-point correction (Hartree):		0.145768	

C4H9O3H.ppppp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92491794

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.108668	0.376736	0.957282
O	0.752057	-0.765831	0.391538
O	1.560563	-0.344495	-0.672948
O	2.745959	0.167743	-0.120002
H	3.249584	-0.636716	0.065906
C	-0.792481	1.099761	-0.027210
H	-0.458287	-0.053627	1.783060
H	0.868402	1.042758	1.369202

C	-1.753268	0.176195	-0.771941	
H	-1.355634	1.845399	0.541003	
H	-0.176349	1.645549	-0.741730	
C	-2.636896	-0.652540	0.153129	
H	-2.377192	0.785245	-1.427676	
H	-1.178336	-0.488691	-1.418223	
H	-3.160691	-0.015686	0.869063	
H	-2.050015	-1.379286	0.715023	
H	-3.386254	-1.205186	-0.411896	
Rotational constants (GHz):				5.9373500 1.3231200 1.3043000
Vibrational harmonic frequencies (cm-1):				
41.1795	64.8518		122.6343	
206.0225	221.9855		293.6195	
361.4679	373.0316		436.9582	
582.2616	615.3856		733.3695	
829.9370	857.8541		913.6060	
954.4939	980.8055		1004.9234	
1045.7931	1105.4378		1135.3590	
1170.2830	1267.5133		1282.8963	
1324.9506	1370.0841		1393.1671	
1407.2292	1417.9497		1420.8247	
1481.0842	1492.8035		1496.6783	
1504.9038	1518.1262		3054.8898	
3057.0182	3069.2507		3080.6340	
3101.1006	3109.1646		3125.4819	
3129.9738	3135.8329		3791.9508	
Zero-point correction (Hartree): 0.145996				

C4H9O3H.ppppt

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E(CCSD(T)/Aug-CC-pVTZ) (Hartree): -383.39299035
E(CCSD/Aug-CC-pVTZ) (Hartree): -383.32911284
T1 diagnostic: 0.013425
E(MP2/Aug-CC-pVTZ) (Hartree): -383.28248451
E(MP3/Aug-CC-pVTZ) (Hartree): -383.32007945
E(RHF/Aug-CC-pVTZ) (Hartree): -381.82816446
E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92518246
Electronic state : 1-A
Cartesian coordinates (Angs):
C -0.375661 1.101317 0.110626
O -1.089530 0.297195 -0.830345
O -1.614036 -0.815000 -0.158135
O -2.792184 -0.395912 0.482343
H -3.432658 -0.404005 -0.242307
C 0.868132 0.420508 0.644742
H -0.122232 1.988788 -0.471924
H -1.059940 1.390693 0.909605
C 1.869850 0.054656 -0.443141
H 1.333507 1.096730 1.367275
H 0.575126 -0.473792 1.198324
C 3.111603 -0.619997 0.124208
H 1.386507 -0.603455 -1.166568
H 2.154943 0.958580 -0.988282
H 2.845939 -1.537964 0.650098
H 3.620062 0.032963 0.835211
H 3.821208 -0.877705 -0.660941
Rotational constants (GHz): 6.4021300 1.1429500 1.1014800
Vibrational harmonic frequencies (cm-1):
37.9346 77.6658 99.0885
186.1094 239.2790 260.3183
305.3855 373.9052 441.1208
570.7462 598.3379 742.9241
837.7828 861.8011 910.9130
957.6707 978.8413 1010.1893
1063.8355 1098.8567 1143.1350
1188.2820 1266.9380 1293.0940
1332.2979 1344.0128 1403.9174
1411.3568 1414.5742 1422.9409
1480.0873 1490.8670 1497.3416
1504.6655 1512.6305 3049.9444
3055.8593 3058.0541 3073.6434
3089.9385 3105.1271 3122.7992
3126.2370 3133.9788 3791.4061
Zero-point correction (Hartree): 0.145725

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C4H9O3H.pppptm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92395424
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.032797	-0.550846	0.153014
O	1.273950	-0.836385	-0.490468
O	2.066851	0.319011	-0.463417
O	2.672688	0.375259	0.802827
H	3.404138	-0.250283	0.707686
C	-0.831319	0.406727	-0.643857
H	-0.427734	-1.534398	0.245370
H	0.236266	-0.169166	1.156934
C	-2.118764	0.773447	0.090732
H	-0.250765	1.307498	-0.843660
H	-1.067414	-0.049660	-1.608033
C	-3.029204	-0.421338	0.357331
H	-1.867084	1.261254	1.035839
H	-2.658561	1.513405	-0.501372
H	-2.575850	-1.127655	1.053059
H	-3.243897	-0.957723	-0.568613
H	-3.978066	-0.104291	0.787934

Rotational constants (GHz): 6.8831600 1.0775000 1.0590000
 Vibrational harmonic frequencies (cm-1):

48.1132	78.5622	116.4002
172.9266	235.0413	288.6354
291.8062	364.3690	428.0975
562.7362	596.3825	750.4837
803.9214	898.6071	912.1703
965.4132	974.1573	1005.3576
1073.7005	1098.7449	1139.5432
1187.1359	1268.7299	1292.2484
1334.2346	1349.0280	1378.4525
1415.1918	1421.4746	1423.5008
1487.3604	1495.4573	1502.0358
1508.3232	1513.8196	3055.0590
3058.9074	3061.3964	3069.8493
3095.4480	3111.0813	3126.5438
3131.9419	3136.4586	3791.7743

Zero-point correction (Hartree): 0.145850

C4H9O3H.ppptp

 E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92366772
 Electronic state : 1-A
 Cartesian coordinates (Angs):

C	0.069055	-0.417752	0.662154
O	1.397348	-0.871425	0.402914
O	1.943937	-0.078583	-0.615603
O	2.407327	1.104527	-0.016306
H	3.253490	0.825402	0.359793
C	-0.885510	-0.736234	-0.471634
H	-0.209040	-0.954476	1.571360
H	0.108470	0.648398	0.889074
C	-2.332660	-0.384135	-0.132591
H	-0.571825	-0.191075	-1.363772
H	-0.802915	-1.800908	-0.696351
C	-2.564085	1.108506	0.083553
H	-2.972482	-0.732438	-0.944361
H	-2.641384	-0.936929	0.758759
H	-2.208640	1.681558	-0.774205
H	-2.042161	1.476572	0.966507
H	-3.623209	1.325431	0.216262

Rotational constants (GHz): 5.2570900 1.2252800 1.1053100
 Vibrational harmonic frequencies (cm-1):

40.7374	68.4642	117.0425
159.5282	234.7023	287.2645
302.2686	368.8340	414.3514
565.0406	597.1977	754.3174
805.4276	899.0425	908.7733
960.9710	982.1792	1001.9049
1069.3655	1099.8179	1138.7679
1192.0173	1269.5758	1290.9642
1333.2555	1351.1335	1378.0317
1416.3453	1420.9065	1424.1910
1488.8531	1494.5467	1502.1917
1508.8575	1513.1448	3051.6895
3062.1389	3065.9532	3076.3705
3093.5519	3105.6114	3128.4385

3130.8597 3137.8426 3791.4070
Zero-point correction (Hartree): 0.145812

C4H9O3H.ppptt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92478083
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.285230	0.779914	0.367004
O	-1.465754	0.841411	-0.431288
O	-1.960601	-0.460164	-0.591601
O	-2.695020	-0.769302	0.565410
H	-3.535391	-0.319972	0.400362
C	0.879038	0.125377	-0.346756
H	-0.075162	1.827826	0.587331
H	-0.522323	0.272392	1.304801
C	2.133520	0.117830	0.518924
H	0.606578	-0.897644	-0.611956
H	1.070705	0.660952	-1.279397
C	3.316194	-0.533950	-0.185480
H	2.390432	1.143662	0.796038
H	1.924827	-0.410584	1.452487
H	3.556593	-0.004835	-1.108364
H	3.087836	-1.567858	-0.446633
H	4.205771	-0.534519	0.443005

Rotational constants (GHz): 6.8972000 1.0101500 0.9794700
Vibrational harmonic frequencies (cm-1):

60.7640	72.9175	117.8435
147.4013	212.8054	249.9116
321.0636	370.4515	405.2146
553.8220	595.6533	740.0889
806.8137	909.6577	922.1671
954.9073	985.8136	1032.2942
1079.3641	1088.0225	1146.9297
1204.1245	1268.8066	1287.7473
1329.3716	1332.8746	1385.0722
1414.9504	1420.0031	1422.4092
1490.5975	1493.4488	1503.2329
1504.2205	1515.8373	3045.5902
3059.1177	3061.2946	3070.6633
3075.8445	3102.7727	3124.0126
3128.8487	3135.5029	3792.3151

Zero-point correction (Hartree): 0.145672

C4H9O3H.pptmm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92452108
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.130594	0.489837	0.612877
O	-0.762892	-0.167936	-0.484534
O	-1.907459	-0.817260	-0.009173
O	-2.927393	0.145097	0.079085
H	-3.237912	0.198154	-0.835176
C	1.120299	1.150830	0.068967
H	-0.818630	1.227706	1.027128
H	0.101458	-0.252843	1.378152
C	2.095661	0.184526	-0.603060
H	0.828839	1.932235	-0.634680
H	1.611677	1.645595	0.910503
C	2.537227	-0.958348	0.303546
H	1.634851	-0.222729	-1.503547
H	2.968862	0.752337	-0.927910
H	1.708561	-1.629803	0.527915
H	2.929497	-0.579889	1.249596
H	3.319191	-1.551045	-0.168981

Rotational constants (GHz): 6.3506700 1.1993100 1.1147700
Vibrational harmonic frequencies (cm-1):

51.8319	58.1034	124.8715
174.0638	235.9124	299.8965
328.5194	379.5479	412.1782
509.4639	622.8907	744.6065
840.6340	860.4260	942.7503
977.6414	998.6995	1009.8246
1043.8930	1113.5332	1149.2897
1173.4068	1253.7096	1278.4719
1322.7681	1372.8805	1390.4823

1411.4791	1420.8640	1422.1150
1477.8958	1495.1211	1503.7612
1510.7009	1535.9774	3056.6233
3059.3729	3068.6368	3072.0734
3098.8786	3107.2553	3120.0808
3128.2680	3136.9170	3793.0522

Zero-point correction (Hartree): 0.146006

C4H9O3H.pptmp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92308165

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.154393	0.791768	0.380549
O	-0.699728	-0.372076	-0.244611
O	-1.911994	-0.678216	0.384453
O	-2.895702	0.153253	-0.177571
H	-3.110341	-0.310643	-0.998428
C	1.159895	1.114221	-0.308241
H	-0.871465	1.605405	0.266241
H	-0.010087	0.583928	1.444020
C	2.351195	0.279300	0.156175
H	1.017258	1.003802	-1.386237
H	1.369873	2.169833	-0.127630
C	2.209340	-1.216048	-0.103709
H	3.245939	0.651308	-0.346478
H	2.506148	0.452088	1.224362
H	2.006044	-1.408041	-1.158126
H	1.386927	-1.642766	0.467674
H	3.122872	-1.744043	0.167790

Rotational constants (GHz): 6.0391800 1.2557500 1.1102200

Vibrational harmonic frequencies (cm-1):

39.9808	76.6648	100.1000
164.9696	250.3538	282.9100
323.4091	367.0759	406.1574
493.1209	617.5013	778.7829
816.9625	869.6164	940.4137
980.1572	992.7042	1010.5870
1045.0798	1116.1629	1142.0365
1180.5668	1255.7305	1293.0988
1313.6201	1378.6607	1390.3587
1416.7249	1420.2416	1423.9884
1474.7123	1491.4259	1503.4855
1509.1220	1525.2118	3050.5096
3054.1653	3059.6810	3064.3826
3088.1059	3104.9147	3113.5341
3130.0911	3146.2482	3792.6070

Zero-point correction (Hartree): 0.145793

C4H9O3H.pptmt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92494459

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.326143	0.651625	0.457234
O	-0.925385	-0.473576	-0.185597
O	-2.215070	-0.640042	0.329667
O	-3.053952	0.264511	-0.343408
H	-3.237050	-0.203061	-1.169799
C	1.078505	0.776379	-0.094196
H	-0.923656	1.537950	0.240374
H	-0.317170	0.473345	1.535069
C	1.976535	-0.405620	0.253127
H	1.024847	0.898267	-1.178818
H	1.510103	1.697595	0.304997
C	3.388201	-0.227965	-0.289239
H	2.007442	-0.521325	1.339536
H	1.536614	-1.321135	-0.143693
H	3.851871	0.672168	0.117279
H	3.376311	-0.131792	-1.375813
H	4.023360	-1.075677	-0.035985

Rotational constants (GHz): 9.3943700 0.9692800 0.9359100

Vibrational harmonic frequencies (cm-1):

52.6750	81.2964	92.6882
162.3545	243.2958	263.4672
304.2967	336.6434	397.8060
516.4299	630.4370	739.3458

843.9206	863.2435	941.7507
982.0547	985.7371	1028.8790
1059.6721	1101.6237	1160.5633
1185.9740	1256.9142	1285.3285
1328.7621	1338.7213	1404.8985
1414.7251	1416.2233	1420.2839
1478.3036	1497.1885	1504.3616
1512.4902	1525.7949	3052.8458
3056.7974	3057.9857	3061.9492
3089.2232	3106.3930	3115.6400
3127.5113	3134.6518	3794.3183

Zero-point correction (Hartree): 0.145701

C4H9O3H.pptpm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92339378

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.069429	-1.053409	0.359327
O	-0.783932	-0.372737	-0.675048
O	-2.121482	-0.262188	-0.281832
O	-2.216240	0.864347	0.554314
H	-2.274236	1.587617	-0.085021
C	1.391736	-1.092271	-0.054919
H	-0.204143	-0.507953	1.296749
H	-0.489811	-2.054714	0.461081
C	2.185829	0.158202	0.316942
H	1.849597	-1.963567	0.415563
H	1.433805	-1.261913	-1.133838
C	1.622984	1.449003	-0.266730
H	2.223095	0.239116	1.406247
H	3.216603	0.025159	-0.016350
H	0.633113	1.662028	0.135551
H	1.526711	1.376305	-1.350721
H	2.271775	2.293395	-0.036459

Rotational constants (GHz): 4.3824500 1.5300400 1.2726200

Vibrational harmonic frequencies (cm-1):

52.1129	84.1979	124.5730
171.6533	258.3724	279.9645
320.5524	367.6352	411.3056
479.5955	621.8062	778.5883
823.0122	868.6369	940.5614
976.5124	994.0789	1014.5771
1042.8671	1114.6293	1143.4327
1179.4385	1256.0069	1290.0245
1313.7159	1377.4183	1387.5028
1415.5007	1419.5394	1424.1749
1477.1567	1491.6161	1501.8479
1508.5943	1524.2310	3052.7871
3058.0753	3060.4069	3062.8350
3090.2685	3106.8731	3110.2124
3131.5142	3138.5841	3791.3805

Zero-point correction (Hartree): 0.145890

C4H9O3H.pptpp

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92490783

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.084265	-0.893411	0.612234
O	-0.835531	-0.588369	-0.562200
O	-2.144665	-0.279168	-0.177095
O	-2.149553	1.067949	0.223489
H	-2.209495	1.531952	-0.622893
C	1.350670	-1.110593	0.174650
H	-0.168436	-0.056160	1.306411
H	-0.501270	-1.787884	1.077403
C	1.961125	0.084578	-0.557903
H	1.929554	-1.327113	1.075943
H	1.400702	-1.998356	-0.457742
C	1.868842	1.386755	0.228797
H	3.006516	-0.142703	-0.772026
H	1.464576	0.205844	-1.521051
H	2.292230	1.272230	1.228706
H	0.833070	1.709369	0.339036
H	2.412312	2.185552	-0.274010

Rotational constants (GHz): 4.2741000 1.5476000 1.2788400

Vibrational harmonic frequencies (cm-1):

56.3042	67.3638	144.2506
176.1927	243.4162	306.8055
334.1223	382.5713	420.1050
501.5714	632.9744	743.6589
839.1967	859.5881	940.7167
978.9901	991.7446	1014.7452
1042.5986	1112.2481	1152.0543
1172.8700	1256.2924	1278.5446
1322.9510	1373.5229	1389.0032
1412.0301	1420.4028	1423.8301
1479.3749	1496.1934	1504.2473
1511.5446	1535.9668	3055.2909
3059.2678	3070.1362	3073.2463
3098.5149	3106.3888	3121.6594
3127.1435	3135.0567	3791.5613

Zero-point correction (Hartree): 0.146159

C4H9O3H.pptpt

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92491773
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.337141	0.874708	0.442505
O	0.989727	0.237204	-0.655535
O	2.362603	0.199669	-0.389247
O	2.595108	-0.907382	0.444389
H	2.613463	-1.638966	-0.187687
C	-1.146806	0.858843	0.141111
H	0.560986	0.316799	1.354358
H	0.721714	1.891562	0.534462
C	-1.747950	-0.541955	0.116916
H	-1.646204	1.460717	0.904332
H	-1.320929	1.356538	-0.816039
C	-3.245735	-0.515535	-0.156461
H	-1.241114	-1.137738	-0.642996
H	-1.553236	-1.028897	1.075837
H	-3.455005	-0.051826	-1.121379
H	-3.771496	0.059108	0.607598
H	-3.667586	-1.519593	-0.169761

Rotational constants (GHz): 6.5663400 1.0757200 1.0063100

Vibrational harmonic frequencies (cm-1):

47.4853	70.0994	113.0774
162.5521	248.3583	268.5779
303.0557	339.7075	407.6020
501.3668	639.3774	736.4078
840.4029	863.5494	942.3549
975.3592	989.1646	1030.6848
1059.7059	1101.7250	1162.0452
1184.9153	1257.0820	1284.9994
1328.2150	1337.6684	1404.1612
1415.1337	1416.5081	1422.5625
1478.8184	1497.3267	1505.3460
1512.7191	1524.1697	3051.7781
3056.7632	3060.1517	3061.8272
3087.7478	3104.8735	3113.8250
3127.0274	3134.6880	3793.7098

Zero-point correction (Hartree): 0.145722

C4H9O3H.ppttm

E(RM062X/Aug-CC-pVTZ) (Hartree): -383.92397299
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.062817	-0.175410	-0.313113
O	1.254234	-0.793793	0.167947
O	2.348738	-0.187953	-0.460062
O	2.626953	0.998383	0.239580
H	3.133394	0.674732	0.997117
C	-1.091231	-0.830512	0.417930
H	0.119095	0.894402	-0.109279
H	-0.009802	-0.334755	-1.392275
C	-2.447599	-0.390920	-0.129096
H	-0.988066	-1.912896	0.326244
H	-1.021709	-0.588574	1.480692
C	-2.696091	1.108855	-0.007735
H	-2.528506	-0.693067	-1.176022

H	-3.227250	-0.932097	0.408371
H	-2.015180	1.682122	-0.636722
H	-2.557100	1.441796	1.022244
H	-3.711655	1.363158	-0.308010
Rotational constants (GHz):			6.1644300 1.0849300 0.9821300
Vibrational harmonic frequencies (cm-1):			
54.3673	69.1588	117.1611	
159.0964	202.7312	277.6087	
309.4980	374.5801	423.4023	
483.3518	613.4155	759.6507	
816.6338	895.4674	940.4345	
971.4174	1004.0797	1012.7634	
1071.4926	1102.4826	1160.3257	
1187.3628	1252.1586	1296.2034	
1315.5015	1354.1468	1379.6160	
1416.9379	1422.1713	1428.3809	
1493.3750	1496.7361	1508.9633	
1513.5256	1529.1011	3053.4576	
3056.2497	3061.2421	3065.6431	
3095.5554	3101.1187	3123.7200	
3129.1302	3137.0574	3792.7798	
Zero-point correction (Hartree): 0.145869			

C4H9O3H.ppttp

E (RM062X/Aug-CC-pVTZ) (Hartree): -383.92392189
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.062158	-0.096551	-0.060786
O	-1.224438	0.606900	-0.494268
O	-2.287300	-0.300527	-0.567418
O	-2.798900	-0.449515	0.732892
H	-3.363299	0.330725	0.820898
C	1.072789	0.907015	-0.050580
H	-0.240589	-0.499253	0.939456
H	0.123240	-0.919176	-0.752653
C	2.353836	0.328128	0.546118
H	1.257275	1.246386	-1.072132
H	0.756873	1.777910	0.525820
C	2.895549	-0.873240	-0.221623
H	3.109298	1.114523	0.567401
H	2.171507	0.047473	1.586222
H	3.022557	-0.631649	-1.278288
H	2.224913	-1.729770	-0.154784
H	3.863239	-1.184153	0.169637
Rotational constants (GHz):			6.9243800 1.0115500 0.9851100
Vibrational harmonic frequencies (cm-1):			
45.4744	74.9531	119.1043	
157.9686	196.0239	278.1593	
310.1748	368.8124	423.1695	
482.2630	613.3076	757.7791	
815.6882	894.2837	941.4055	
968.4796	1005.0187	1010.9357	
1071.6638	1102.0403	1160.1928	
1186.9555	1251.7095	1294.7931	
1314.0794	1353.0410	1377.4985	
1415.5494	1421.1493	1427.4235	
1492.5017	1496.1017	1508.1882	
1513.6339	1531.1382	3056.7407	
3057.0719	3061.4785	3066.4666	
3095.7485	3099.5387	3122.3521	
3128.9531	3137.0674	3794.1177	
Zero-point correction (Hartree): 0.145803			

C4H9O3H.ppttt

E (RM062X/Aug-CC-pVTZ) (Hartree): -383.92477833
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.254082	0.091079	0.393303
O	-1.272009	-0.738332	-0.162051
O	-2.501297	-0.350855	0.383482
O	-2.947367	0.765241	-0.344406
H	-3.333008	0.355292	-1.130721
C	1.060164	-0.358303	-0.207261
H	-0.468458	1.132117	0.143021
H	-0.256733	-0.025444	1.479340

C	2.230363	0.457129	0.331255	
H	1.212152	-1.417084	0.013471	
H	1.009124	-0.261951	-1.293934	
C	3.559670	0.015631	-0.266549	
H	2.062818	1.515293	0.117044	
H	2.266246	0.363395	1.419173	
H	3.552044	0.125915	-1.351544	
H	3.756182	-1.033232	-0.041441	
H	4.388326	0.604053	0.124906	
Rotational constants (GHz):		10.1241700	0.8756800	0.8558600
Vibrational harmonic frequencies (cm-1):				
54.7474	76.9629		129.9719	
134.7520	176.0919		252.8498	
318.3738	359.5466		398.7403	
484.4333	621.0996		743.3997	
819.7482	913.1504		942.9867	
962.2134	1008.7473		1051.6602	
1079.5792	1090.6558		1165.4732	
1196.6602	1253.4488		1297.0441	
1312.0499	1329.3250		1387.7780	
1415.8564	1419.9239		1425.2761	
1493.5064	1500.5515		1504.7304	
1513.5396	1531.0400		3050.9937	
3055.7860	3060.6146		3066.0660	
3079.6995	3096.6215		3118.2724	
3129.6483	3135.9306		3790.7643	
Zero-point correction (Hartree): 0.145690				