Supporting Information

Simultaneous Quantification of H_2O_2 and Organic Hydroperoxides by ^1H NMR Spectroscopy

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Synthesis of organic peroxides

Preparation of hydroxymethyl hydroperoxide (HMHP). The procedure reported by O'Sullivan *et al.*[1] was slightly modified. NaOH (220 μL, 0.1 M), H_2O_2 (53.8 μL, 9.3 M), and formaldehyde (37.3 μL, 13.4 M) were added to stirring milli-Q water (100 mL), resulting in a solution at pH 10. For quantification, 10-μL samples of this solution were diluted 50-fold using 1 mM 2-(N-morpholino)ethanesulfonic acid (MES) buffer containing 2% D_2O at pH 6.

Preparation of benzyl hydroperoxide ($PhCH_2OOH$). A homogenous mixture of benzyl chloride (1.0 mmol, 126 mg), H_2O_2 (1.0 mmol, 30%, 102 μL), KOH (1.2 mmol, 40%, 140 mg), and methanol (2 mL) were left at room temperature in a 15-mL falcon tube for two days. The formed solid was then removed by centrifugation and the concentration of the methanolic $PhCH_2OOH$ solution was determined to be 17.2 mM after 50-fold dilution by 1 mM MES containing 2% D_2O at pH 6.0.

Preparation of isopropyl hydroperoxide (*i*-PrOOH). A mixture of isopropyl chloride (1.0 mmol, 76 mg), H_2O_2 (1.0 mmol, 30%, 102 μL), KOH (1.2 mmol, 40% 140 mg), and methanol (1 mL) was stirred at room temperature in a 15-mL falcon tube for two days. The concentration of *i*-PrOOH in the methanol solution was determined to be 1.2 mM after 50-fold dilution by 1 mM MES containing 2% D_2O at pH 6.0.

Preparation of methyl hydroperoxide (MeOOH) and ethyl hydroperoxide (EtOOH). The procedure reported by O'Sullivan *et al.*[1] was slightly modified. KOH (2.0 mL, 40%, 20 mmol) was added to a stirring mixture of dimethyl sulfate (0.95 mL, 10 mmol), H_2O_2 (2.04 mL, 30%, 20 mmol) and water (30 mL) in an ice-bath. The mixture was then immersed into a water bath set to 65 °C while bubbling N_2 gas into it at a rate of 0.25 L/min. The exiting stream of N_2 was then bubbled into an ice-cold water solution (20 mL) using a bubbler with porous fritted glass to increase the MeOOH collection efficiency. After about 50 minutes, when the temperature had reached 50 °C and the bubbling was significantly slower, the reaction was stopped. After 50-fold dilution with 1 mM MES pH 6 buffer, the concentration of the original aqueous stock solution was 1.0 mM. For preparation of the EtOOH stock solution, dimethyl sulfate was replaced by diethyl sulfate (1.31 mL, 10 mmol), and the reaction was stopped after 60 minutes, resulting in a solution containing 0.22 mM EtOOH.

Preparation of *tert*-Amyl hydroperoxide (*t*-AmylOOH). The method reported by Milas and Surgenor[2] was slightly modified as follows. *Tert*-Amyl alcohol (8.8 g, 0.1 mmol) was added to stirring, ice-cold sulfuric acid (14 g, 70%, 0.1 mmol) followed by addition of H_2O_2 (12.3 g, 30%, 0.1 mmol) each over a course of *ca* 2 minutes. The reaction mixture was then kept in a fridge at 5 °C without stirring for 12 h. The organic layer was then neutralized by *ca* 1 g sodium carbonate. After bubbling ended, the mixture was centrifuged and *ca* 1 μL of supernatant was added to 0.5 mL MES buffer stock solution, resulting in a *ca* 11 mM aqueous stock solution as indicated by NMR measurement.

Table S1. Thermodynamic and NMR parameters calculated for individual conformers.

Compound/ Conformer	Relative Free Energy (kcal/mol)	Boltzmann Population (%)	Isotropic Shielding (ppm)	Chemical Shift vs DSS (ppm)
DSS				
1	0.00	85.0	31.646	0.000
2	1.12	11.1	31.639	0.007
3	1.72	3.7	31.664	-0.018
4	3.04	0.3	31.613	0.033
HP				
	0.00	100.0	23.963	7.683
HMHP				
1	0.00	32.9	22.946	8.699
2	0.13	25.9	22.572	9.074
3	0.15	25.1	23.516	8.129
4	0.41	15.5	23.284	8.361
5	2.51	0.3	23.663	7.983
6	2.59	0.3	23.729	7.916
MeOOH				
	0.00	100.0	23.353	8.292
$PhCH_2OOH$				
1	0.00	39.2	23.619	8.026
2	0.06	35.1	23.137	8.508
3	0.23	25.7	23.662	7.984
EtOOH				
1	0.00	55.0	23.390	8.255
2	0.39	27.0	23.438	8.207
3	0.61	18.1	24.053	7.592
***i*-PrOOH**				
1	0.00	47.0	23.978	7.667
2	0.04	43.4	23.488	8.158
3	0.86	9.7	24.426	7.219
***t*-BuOOH**				
	0.00	100.0	24.220	7.426
***t*-AmylOOH**				
1	0.00	26.7	24.350	7.295
2	0.09	22.6	24.288	7.358
3	0.47	11.3	24.432	7.213
4	0.48	11.1	24.249	7.397
5	0.54	10.0	24.368	7.278
6	0.59	9.1	24.318	7.327
7	0.65	8.2	24.273	7.373
8	1.96	0.8	24.172	7.473
9	2.34	0.4	24.166	7.479

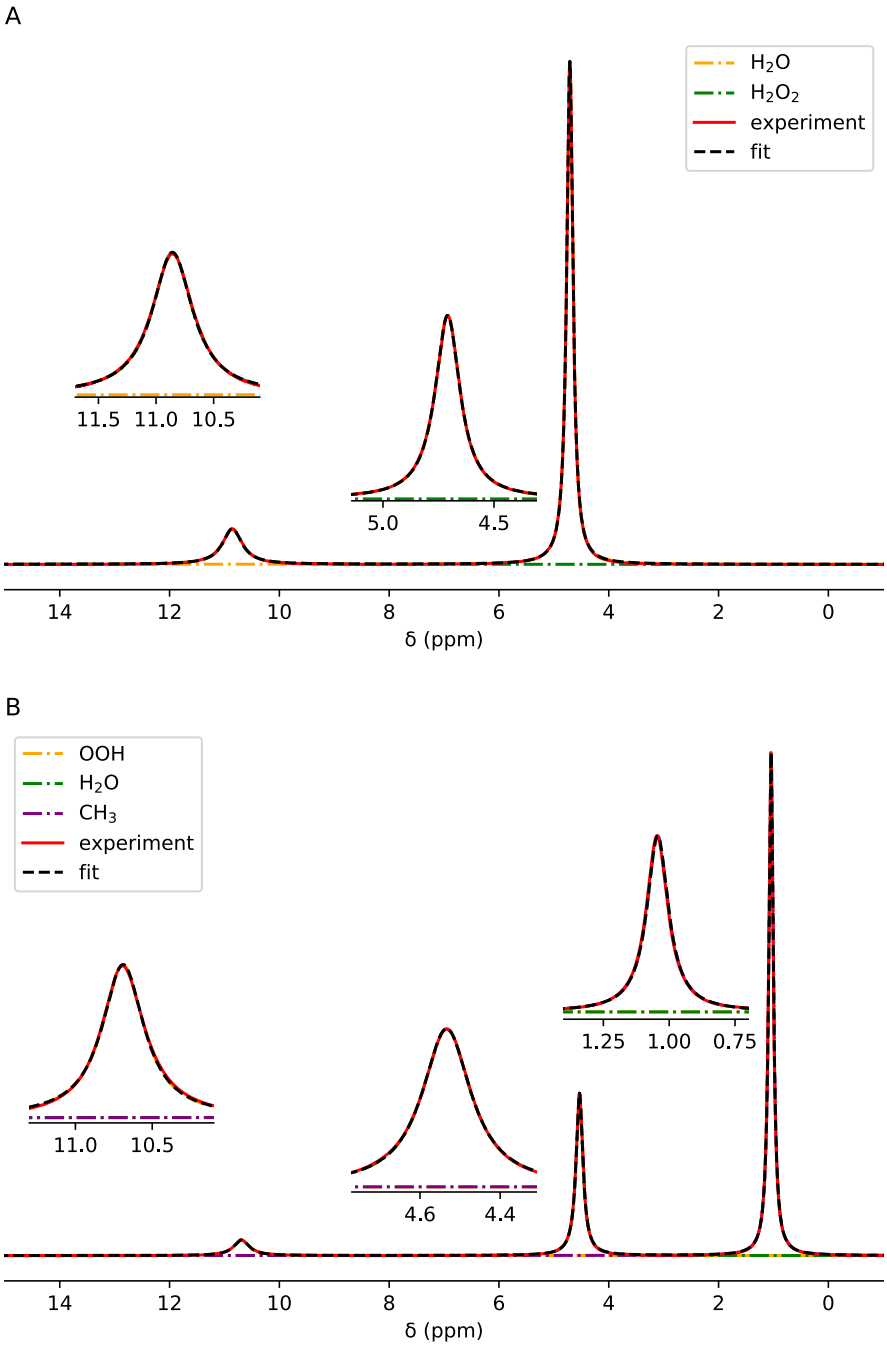

Figure S1. ^{1}H NMR spectra of commercial peroxides. (A) 30% w/w H_2O_2 and (B) 70% w/w *t*-BuOOH. The H_2O_2 sample contains 2% D_2O v/v but since the *t*-BuOOH is saturated with water, a capillary containing D_2O was used to provide the lock signal. Both spectra were recorded at 2 °C. To avoid radiation damping and spectral distortion from receiver overload, the probe was detuned, the receiver gain was decreased to its minimum, and a short excitation pulse of 1 μs (*ca* 4º flip angle) was used; a single scan with an acquisition time of 1 s was recorded and Fourier transformed. Time domain data were apodized by multiplication with an exponential decay function that corresponds to 30 Hz line broadening.

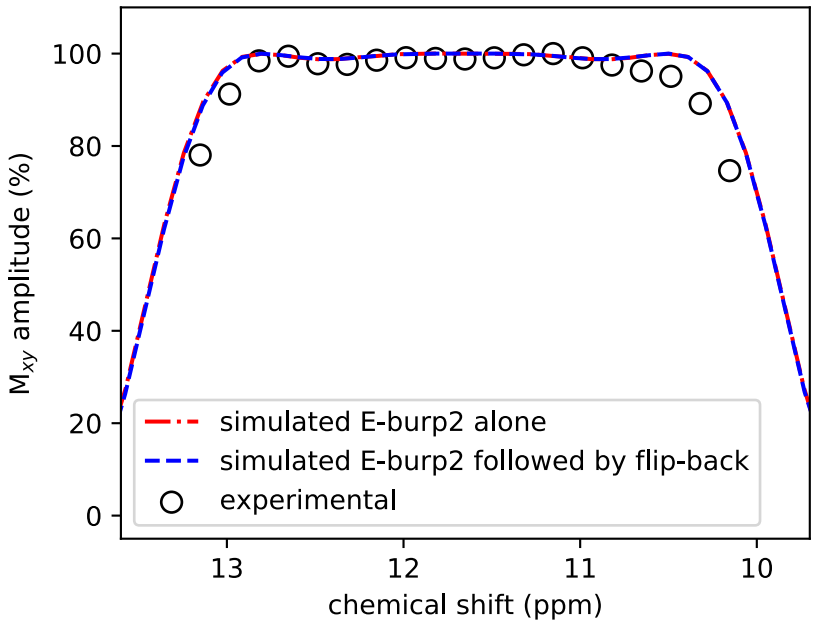

Figure S2. Offset dependence of the total transverse magnetization generated by an *E-BURP2* pulse (red), an *E-BURP2* pulse followed by a water flip-back pulse (blue), and their comparison with experiment. The NMRSim module of Bruker Topspin-3 software was used for the simulations. For experimental measurements, a 10 mM *t*-BuOOH sample in 1 mM MES adjusted to pH 6.0 containing 2% v/v D_2O was used. The *E-BURP2* pulse was first centered at the *t*-BuOOH resonance (11.66 ppm) and a reference spectrum was recorded. The center of the *E-BURP2* pulse was then stepped in 100 Hz increments while the intensity of the *t*-BuOOH peak was compared to the reference spectrum.

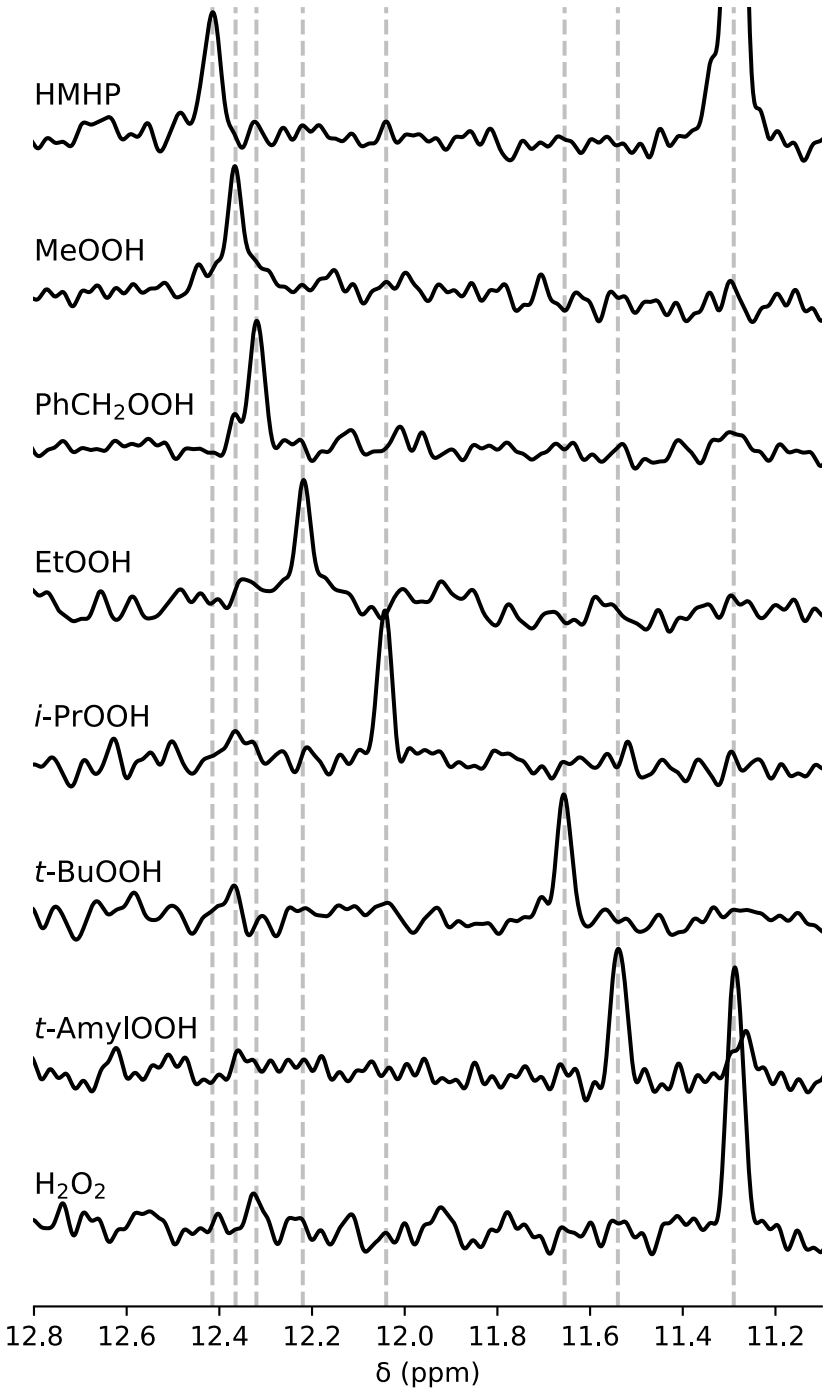

Figure S3. NMR spectra of individual OHP species (1 μM analyte, 1 mM MES; pH 6; 2 °C).

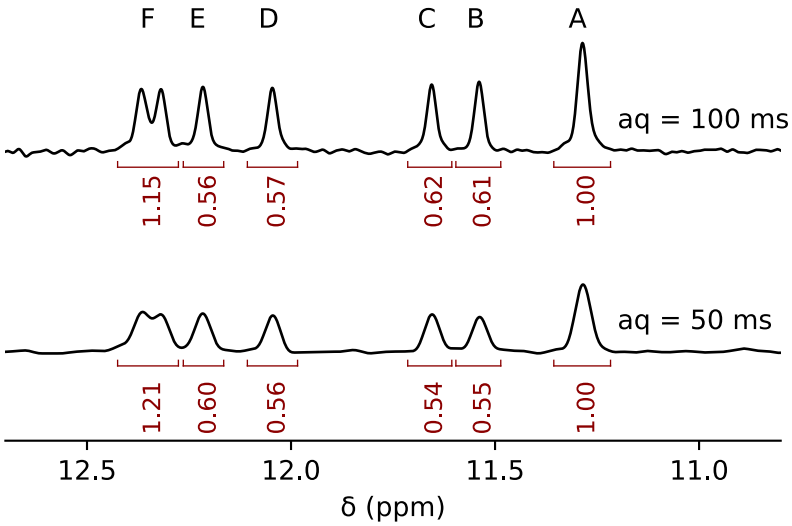

Figure S4. Comparison of the integrated areas of various hydroperoxides, recorded with acquisition times of 100 ms (top) and 50 ms (bottom), relative to those of an internal 1 μM H_2O_2 reference signal. A, B, C, D, and E are H_2O_2, *t*-AmylOOH, *t*-BuOOH, *i*-PrOOH, EtOOH, and F is the combined $PhCH_2OOH$ and MeOOH signals. Each spectrum results from 32k transients. FIDs were apodized with a π/2-shifted, squared sine-bell function prior to Fourier transformation. The integration tool was used as implemented in Bruker Topspin-4.

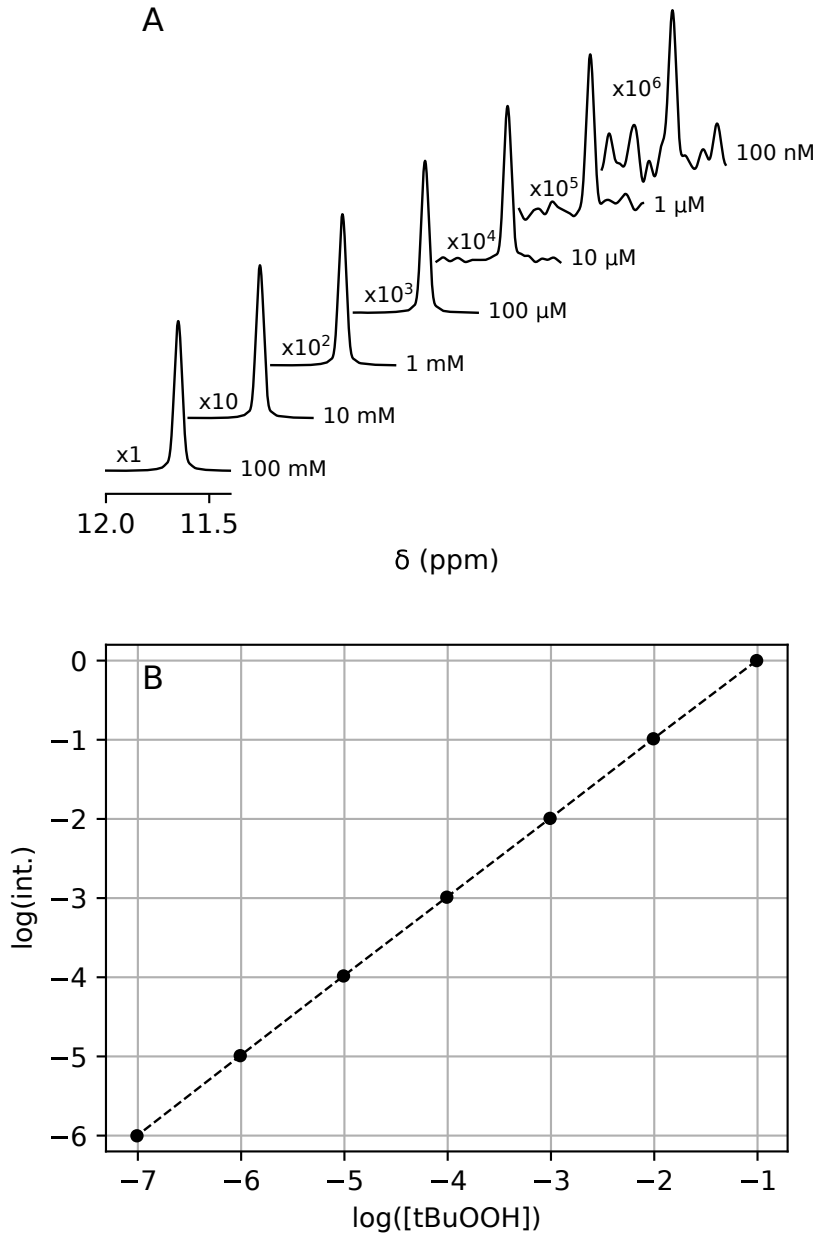

Figure S5. Resonance intensity versus concentration of *t*-BuOOH. (A) Downfield region of *t*-BuOOH ^{1}H NMR spectra over six orders of magnitude of concentration range and (B) decadic logarithm correlation between the peak intensity and concentration. Samples were prepared by sequential dilution of a 100 mM stock solution of commercial 70% w/w *t*-BuOOH (Sigma-Aldrich). All samples contained 1 mM MES and 2% D_2O v/v at pH 6.0. Spectra were collected at 2 °C. Spectra result from 1024 FIDs except for the 1.0 and 0.1 µM samples for which 16k and 200k FIDs were recorded, respectively, and have been scaled accordingly.

Bruker Pulse Program

```
#include <Avance.incl>
"acqt0=-p1*2/3.1416"

1 ze
2 10u
  d1
  (p10:sp10 ph1) ; 2.5 ms E-Burp2 pulse
  3u
  3u pl1:f1
  (p1 ph1:r):f1  ; water flip-back pulse.
  4u
  go=2 ph31
  10u mc #0 to 2 F0(zd)
exit

ph1=0 2 2 0
ph31=0 2 2 0
```

Optimized coordinates and calculated thermodynamic parameters

Abbreviations:	
NImag	Number of Imaginary Frequencies
PG	Point Group Symmetry
HMHP	Hydroxymethyl Hydroperoxide
Units:	
Energy	Atomic Units (Hartree per particle; 1 Atomic Unit = 627.51 kcal/mol)
Cartesian Coordinates	Angstroms
Temperature	Kelvin
Pressure	Atm

(H_2O_2, PG = C_2, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.026050 E(Thermal)=                  0.029001
 E(QCISD(T))=             -151.166253 E(Empiric)=                 -0.066304
 DE(MP2)=                   -0.197702 DE(HF)=                     -0.018616
 G4MP2(0 K)=              -151.422825 G4MP2 Energy=             -151.419874
 G4MP2 Enthalpy=          -151.419003 G4MP2 Free Energy=        -151.442504
Cartesian coordinates:
O         -0.000000   -0.721704   -0.070790
O         -0.000000    0.721704   -0.070790
H         -0.704046   -0.917684    0.566316
H          0.704046    0.917684    0.566316
```

(MeOOH, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.053892 E(Thermal)=                  0.057696
 E(QCISD(T))=             -190.337772 E(Empiric)=                 -0.094720
 DE(MP2)=                   -0.246646 DE(HF)=                     -0.021371
 G4MP2(0 K)=              -190.646617 G4MP2 Energy=             -190.642813
 G4MP2 Enthalpy=          -190.641941 G4MP2 Free Energy=        -190.669600
Cartesian coordinates:
O         -1.183459   -0.226947   -0.121673
O         -0.018681    0.613267    0.025129
C          1.122593   -0.232331   -0.002251
H         -1.400883   -0.427396    0.803480
H          1.976221    0.448040    0.077887
H          1.181754   -0.791095   -0.942553
H          1.124471   -0.926127    0.847048
```

(EtOOH, conformer 1, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.081734 E(Thermal)=                  0.086623
 E(QCISD(T))=             -229.524606 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.299764 DE(HF)=                     -0.025285
 G4MP2(0 K)=              -229.891057 G4MP2 Energy=              -229.886167
 G4MP2 Enthalpy=          -229.885296 G4MP2 Free Energy=         -229.916180
Cartesian coordinates:
O         -1.823071    0.063462   -0.098888
O         -0.514645   -0.536818   -0.004429
C          1.818097   -0.146926    0.018888
C          0.453152    0.516641   -0.021216
H         -2.046804    0.202072    0.835716
H          2.593343    0.624513    0.009607
H          1.964689   -0.794191   -0.850751
H          1.938011   -0.745349    0.926725
H          0.325129    1.114952   -0.931018
H          0.299867    1.166561    0.850227
```

(EtOOH, conformer 2, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.081878 E(Thermal)=                  0.086605
 E(QCISD(T))=             -229.525070 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.299049 DE(HF)=                     -0.025207
 G4MP2(0 K)=              -229.890584 G4MP2 Energy=              -229.885857
 G4MP2 Enthalpy=          -229.884985 G4MP2 Free Energy=         -229.915559
Cartesian coordinates:
O          1.467671   -0.495140    0.221131
O          0.713828    0.579854   -0.384923
C         -1.471988   -0.528785   -0.086218
C         -0.566108    0.643046    0.252398
H         -2.450141   -0.384167    0.383452
H         -1.616861   -0.609768   -1.168101
H         -1.055266   -1.469439    0.284969
H         -0.976446    1.584601   -0.130329
H         -0.425550    0.743732    1.335220
H          1.300844   -1.228240   -0.391954
```

(EtOOH, conformer 3, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.081888 E(Thermal)=                  0.086599
 E(QCISD(T))=             -229.524715 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.299089 DE(HF)=                     -0.025202
 G4MP2(0 K)=              -229.890254 G4MP2 Energy=              -229.885543
 G4MP2 Enthalpy=          -229.884672 G4MP2 Free Energy=         -229.915210
Cartesian coordinates:
O          1.420726   -0.602766    0.057598
O          0.701495    0.563226   -0.403859
C         -1.501316   -0.508269   -0.087152
C         -0.554095    0.620307    0.280705
H         -2.460121   -0.362613    0.420935
H         -1.681638   -0.528001   -1.166394
H         -1.097036   -1.476162    0.219970
H         -0.952839    1.591119   -0.035961
H         -0.373991    0.660510    1.362678
H          1.920316   -0.240755    0.807543
```

($PhCH_2OOH$, conformer 1, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.133918	E(Thermal)=	0.141262
E(QCISD(T))=	-420.707665	E(Empiric)=	-0.227328
DE(MP2)=	-0.490083	DE(HF)=	-0.042730
G4MP2(0 K)=	-421.333887	G4MP2 Energy=	-421.326543
G4MP2 Enthalpy=	-421.325672	G4MP2 Free Energy=	-421.364902

Cartesian coordinates:

O	2.450568	-0.022878	1.199468
O	2.431774	-0.435140	-0.186059
C	-2.603381	-0.198001	0.339096
C	-2.082551	1.089190	0.231238
C	-1.792067	-1.298813	0.059346
C	-0.754133	1.274539	-0.151168
C	-0.469730	-1.110746	-0.330722
C	1.489052	0.383395	-0.881620
C	0.061020	0.179147	-0.438910
H	-3.635182	-0.345254	0.640504
H	-2.705857	1.949732	0.451113
H	-2.192617	-2.303910	0.142285
H	-0.345818	2.277908	-0.227728
H	3.161796	0.638392	1.195399
H	1.779640	1.437335	-0.801264
H	1.629998	0.065162	-1.922373
H	0.160046	-1.967481	-0.548780

($PhCH_2OOH$, conformer 2, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.134181	E(Thermal)=	0.141519
E(QCISD(T))=	-420.707291	E(Empiric)=	-0.227328
DE(MP2)=	-0.490696	DE(HF)=	-0.042860
G4MP2(0 K)=	-421.333994	G4MP2 Energy=	-421.326656
G4MP2 Enthalpy=	-421.325785	G4MP2 Free Energy=	-421.364804

Cartesian coordinates:

O	3.517437	-0.092791	-0.305633
O	2.099667	-0.053118	-0.580596
C	-2.776175	-0.008777	-0.291192
C	-2.104937	1.203663	-0.138526
C	-2.089548	-1.210418	-0.119639
C	-0.750012	1.213303	0.184354
C	-0.735306	-1.198078	0.204438
C	-0.055621	0.013482	0.362213
C	1.413980	0.023007	0.682755
H	-3.832190	-0.017466	-0.539921
H	-2.636429	2.140457	-0.268600
H	-2.609453	-2.155620	-0.234910
H	-0.225512	2.156030	0.306026
H	-0.199591	-2.132192	0.342653
H	3.748095	0.850487	-0.316028
H	1.705715	0.946302	1.196653
H	1.698248	-0.837810	1.297539

($PhCH_2OOH$, conformer 3, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.134267 E(Thermal)=                  0.141420
 E(QCISD(T))=             -420.708452 E(Empiric)=                 -0.227328
 DE(MP2)=                   -0.489985 DE(HF)=                     -0.042670
 G4MP2(0 K)=              -421.334169 G4MP2 Energy=              -421.327015
 G4MP2 Enthalpy=          -421.326144 G4MP2 Free Energy=         -421.364535
Cartesian coordinates:
O          2.499618   -0.023295    1.191544
O          2.449620   -0.375474   -0.209062
C         -2.584220   -0.246589    0.309785
C         -2.089521    1.055161    0.275330
C         -1.749028   -1.313819   -0.023141
C         -0.763361    1.288344   -0.087172
C         -0.428583   -1.077880   -0.394770
C          1.503489    0.483134   -0.850319
C          0.075689    0.227123   -0.430588
H         -3.614328   -0.430751    0.596197
H         -2.731795    1.889445    0.537524
H         -2.128993   -2.329856    0.002940
H         -0.375298    2.302360   -0.105338
H          1.816893   -0.601434    1.569443
H          1.779484    1.530523   -0.687198
H          1.654004    0.245261   -1.910890
H          0.219345   -1.908244   -0.657280
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($PhCH_2OOH$, PG = C_1, NImag = 1)

```
Imaginary frequency (1/cm): -10.8848

Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.134076 E(Thermal)=                  0.140510
 E(QCISD(T))=             -420.708383 E(Empiric)=                 -0.227328
 DE(MP2)=                   -0.490273 DE(HF)=                     -0.042664
 G4MP2(0 K)=              -421.334573 G4MP2 Energy=              -421.328138
 G4MP2 Enthalpy=          -421.327267 G4MP2 Free Energy=         -421.363661
Cartesian coordinates:
O         -2.470359   -0.600028   -1.042262
O         -2.421597    0.495976   -0.103079
C         -1.521158    0.136331    0.955224
C         -0.083451    0.067288    0.507238
C          2.574714   -0.051233   -0.366898
C          1.912019   -1.216290    0.012461
C          1.909955    1.174886   -0.313143
C          0.589593    1.232717    0.122197
C          0.587316   -1.155700    0.443856
H         -1.844416   -0.808567    1.404524
H         -1.753569   -0.372434   -1.656397
H         -1.675824    0.944877    1.678610
H          3.605474   -0.096012   -0.702519
H          2.423742   -2.172116   -0.028839
H          2.423710    2.084807   -0.605399
H          0.073398    2.186976    0.168369
H          0.069197   -2.063114    0.738763
```

(*i*-PrOOH, conformer 1, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.109113 E(Thermal)=                  0.115044
 E(QCISD(T))=             -268.712320 E(Empiric)=                 -0.151552
 DE(MP2)=                   -0.352640 DE(HF)=                     -0.028965
 G4MP2(0 K)=              -269.136365 G4MP2 Energy=             -269.130434
 G4MP2 Enthalpy=          -269.129562 G4MP2 Free Energy=        -269.163092
Cartesian coordinates:
O          1.930796   -0.058467    0.023890
O          0.676248   -0.657925   -0.363679
C         -1.631074   -0.819996   -0.007208
C         -0.523847    1.466546   -0.094212
C         -0.398194    0.009497    0.329624
H         -2.501534   -0.405281    0.508391
H         -1.828424   -0.800720   -1.083960
H         -1.504188   -1.859390    0.308087
H         -1.338791    1.946014    0.456972
H         -0.740716    1.538577   -1.165393
H         -0.189864   -0.053517    1.406142
H          2.168525   -0.586056    0.803442
H          0.397331    2.015226    0.115408
```

(*i*-PrOOH, conformer 2, PG = C1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.109354 E(Thermal)=                  0.115169
 E(QCISD(T))=             -268.712675 E(Empiric)=                 -0.151552
 DE(MP2)=                   -0.352573 DE(HF)=                     -0.028967
 G4MP2(0 K)=              -269.136413 G4MP2 Energy=             -269.130598
 G4MP2 Enthalpy=          -269.129727 G4MP2 Free Energy=        -269.163023
Cartesian coordinates:
O         -1.921393   -0.216424   -0.169530
O         -0.654146   -0.711316    0.315625
C          1.670018   -0.757359    0.034318
C          0.447841    1.470816    0.097360
C          0.409053    0.011762   -0.338520
H         -2.156589    0.435675    0.509074
H         -0.490559    1.977997   -0.143045
H          2.534059   -0.298460   -0.453949
H          1.834450   -0.733737    1.116484
H          1.603249   -1.800160   -0.288138
H          1.255624    1.994170   -0.423374
H          0.623971    1.547417    1.175745
H          0.238633   -0.052295   -1.420508
```

(*i*-PrOOH, conformer 3, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.109229	E(Thermal)=	0.115057
E(QCISD(T))=	-268.711905	E(Empiric)=	-0.151552
DE(MP2)=	-0.352037	DE(HF)=	-0.028858
G4MP2(0 K)=	-269.135122	G4MP2 Energy=	-269.129294
G4MP2 Enthalpy=	-269.128423	G4MP2 Free Energy=	-269.161714

Cartesian coordinates:

O	-1.625837	-0.153513	-0.501823
O	-0.888157	-0.103147	0.742723
C	1.054158	-1.209240	-0.279385
C	0.858284	1.332420	-0.219463
C	0.523216	0.011195	0.462797
H	-1.857387	0.779330	-0.632185
H	2.145930	-1.163111	-0.336333
H	1.943777	1.457390	-0.275019
H	0.921749	0.017854	1.485350
H	0.775511	-2.129664	0.242291
H	0.661714	-1.251386	-1.299170
H	0.462536	1.361916	-1.239064
H	0.444179	2.174705	0.343241

(*t*-BuOOH, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.136223	E(Thermal)=	0.143214
E(QCISD(T))=	-307.900047	E(Empiric)=	-0.179968
DE(MP2)=	-0.405896	DE(HF)=	-0.032545
G4MP2(0 K)=	-308.382232	G4MP2 Energy=	-308.375242
G4MP2 Enthalpy=	-308.374370	G4MP2 Free Energy=	-308.410161

Cartesian coordinates:

O	1.984202	0.124890	-0.167410
O	0.736552	0.022630	-0.889984
C	-1.576468	-0.076074	-0.924398
C	-0.420031	1.284494	0.860833
C	-0.387257	-0.002322	0.035845
C	-0.312429	-1.245864	0.922689
H	-2.507511	-0.096554	-0.351579
H	-1.597600	0.795307	-1.585503
H	-1.528585	-0.980858	-1.537426
H	-1.312891	1.301029	1.492935
H	-1.199590	-1.305935	1.559913
H	-0.445430	2.160721	0.205631
H	-0.265537	-2.153050	0.311942
H	2.245434	-0.805748	-0.088211
H	0.566494	-1.214842	1.572402
H	0.456287	1.358362	1.509230

(*t*-AmylOOH, conformer 1, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164275	E(Thermal)=	0.172417
E(QCISD(T))=	-347.080893	E(Empiric)=	-0.208384
DE(MP2)=	-0.459714	DE(HF)=	-0.036428
G4MP2(0 K)=	-347.621145	G4MP2 Energy=	-347.613003
G4MP2 Enthalpy=	-347.612132	G4MP2 Free Energy=	-347.650705

Cartesian coordinates:

O	-0.862932	1.881593	-0.160496
O	-0.592170	0.661589	-0.887328
C	-1.499264	-0.676813	0.949405
C	-0.298254	-0.425384	0.036239
C	-0.095073	-1.599783	-0.925059
C	2.211709	0.237125	0.055607
C	0.960247	-0.110668	0.865089
H	-2.400610	-0.860303	0.356487
H	-1.681561	0.176986	1.606496
H	-1.315800	-1.554810	1.576033
H	-1.018235	-1.810950	-1.472500
H	3.031446	0.515066	0.725587
H	2.555397	-0.605092	-0.552599
H	2.031444	1.082595	-0.616589
H	1.157964	-0.978990	1.503816
H	0.722466	0.717977	1.541010
H	0.696296	-1.394521	-1.650031
H	0.179621	-2.492897	-0.357005
H	0.006199	2.312621	-0.165807

(*t*-AmylOOH, conformer 2, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164286	E(Thermal)=	0.172450
E(QCISD(T))=	-347.080588	E(Empiric)=	-0.208384
DE(MP2)=	-0.459616	DE(HF)=	-0.036444
G4MP2(0 K)=	-347.620747	G4MP2 Energy=	-347.612583
G4MP2 Enthalpy=	-347.611712	G4MP2 Free Energy=	-347.650560

Cartesian coordinates:

O	1.079418	-1.756287	-0.175059
O	0.662514	-0.572147	-0.891625
C	-2.182409	-0.563439	0.048593
C	-0.991251	-0.052561	0.861894
C	-0.169051	1.588827	-0.917168
C	1.355612	0.875608	0.955352
C	0.206867	0.452542	0.037920
H	-2.950107	-0.968447	0.715612
H	-2.648014	0.230716	-0.543058
H	-1.883239	-1.361913	-0.637314
H	-1.309479	0.769978	1.512877
H	-0.905416	1.264171	-1.656370
H	-0.634875	-0.848247	1.524044
H	-0.595019	2.419048	-0.347028
H	2.225165	1.183376	0.365908
H	2.031009	-1.601209	-0.069930
H	1.653866	0.060060	1.619816
H	1.047000	1.720808	1.577535
H	0.715048	1.953270	-1.448157

(*t*-AmylOOH, conformer 3, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164082	E(Thermal)=	0.172330
E(QCISD(T))=	-347.079734	E(Empiric)=	-0.208384
DE(MP2)=	-0.459589	DE(HF)=	-0.036451
G4MP2(0 K)=	-347.620077	G4MP2 Energy=	-347.611828
G4MP2 Enthalpy=	-347.610957	G4MP2 Free Energy=	-347.649954

Cartesian coordinates:

O	1.961430	-1.069683	-0.244150
O	0.586871	-0.825106	-0.616980
C	-2.297843	-0.687742	-0.064618
C	-1.362850	0.449384	-0.485114
C	0.880183	1.591380	-0.424847
C	0.152768	0.212753	1.562329
C	0.084010	0.371679	0.042295
H	-3.273676	-0.566391	-0.545594
H	-2.464467	-0.701587	1.016572
H	-1.901348	-1.664191	-0.357632
H	-1.771849	1.408738	-0.149568
H	-1.313488	0.498710	-1.579201
H	-0.371176	1.041207	2.048436
H	-0.310099	-0.723478	1.885750
H	1.933291	1.497237	-0.148864
H	1.859902	-1.682729	0.500632
H	1.189566	0.222247	1.908536
H	0.812647	1.704080	-1.511461
H	0.486686	2.499737	0.041168

(*t*-AmylOOH, conformer 4, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164413	E(Thermal)=	0.172549
E(QCISD(T))=	-347.079596	E(Empiric)=	-0.208384
DE(MP2)=	-0.460122	DE(HF)=	-0.036406
G4MP2(0 K)=	-347.620095	G4MP2 Energy=	-347.611959
G4MP2 Enthalpy=	-347.611088	G4MP2 Free Energy=	-347.649936

Cartesian coordinates:

O	2.402808	0.051127	-0.283788
O	1.108700	-0.073971	-0.913861
C	-2.545723	-0.049834	-0.124383
C	-1.193932	-0.117337	-0.839492
C	0.156010	-1.130649	1.072501
C	0.099333	1.383006	0.767811
C	0.039368	0.021845	0.074904
H	-3.355132	-0.156955	-0.853289
H	-2.688842	0.905704	0.388930
H	-2.658373	-0.850573	0.612719
H	-1.141521	0.675046	-1.595029
H	-1.111026	-1.070977	-1.373430
H	-0.709483	1.480272	1.496836
H	-0.662051	-1.097902	1.796719
H	2.636628	-0.876408	-0.124130
H	1.093990	-1.066813	1.630716
H	1.046035	1.501310	1.300213
H	0.121225	-2.095063	0.555495
H	0.006155	2.192924	0.037394

(*t*-AmylOOH, conformer 5, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164393	E(Thermal)=	0.172521
E(QCISD(T))=	-347.079579	E(Empiric)=	-0.208384
DE(MP2)=	-0.460010	DE(HF)=	-0.036410
G4MP2(0 K)=	-347.619990	G4MP2 Energy=	-347.611862
G4MP2 Enthalpy=	-347.610991	G4MP2 Free Energy=	-347.649845

Cartesian coordinates:

O	1.998564	-1.047281	-0.169801
O	1.376684	0.184134	-0.600295
C	-2.293196	-0.761592	0.024333
C	-0.848619	-0.803129	-0.482727
C	-0.367048	1.698252	-0.550320
C	0.196417	0.385409	1.530589
C	0.059207	0.338437	0.008035
H	-2.860218	-1.600304	-0.392309
H	-2.805783	0.159479	-0.270575
H	-2.344778	-0.841041	1.114630
H	-1.353066	1.969424	-0.166008
H	-0.843709	-0.781167	-1.579081
H	-0.754054	0.662697	1.993563
H	-0.417059	1.672701	-1.643029
H	-0.390176	-1.750534	-0.182866
H	2.504296	-0.754097	0.604154
H	0.943226	1.132139	1.818839
H	0.497974	-0.584935	1.934479
H	0.340800	2.476548	-0.250487

(*t*-AmylOOH, conformer 6, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164188	E(Thermal)=	0.172383
E(QCISD(T))=	-347.079688	E(Empiric)=	-0.208384
DE(MP2)=	-0.459619	DE(HF)=	-0.036451
G4MP2(0 K)=	-347.619953	G4MP2 Energy=	-347.611759
G4MP2 Enthalpy=	-347.610887	G4MP2 Free Energy=	-347.649763

Cartesian coordinates:

O	-1.919993	-1.155455	-0.033437
O	-0.576770	-0.898738	-0.500220
C	-0.917391	1.519412	-0.510178
C	-0.099152	0.335204	1.565129
C	-0.080947	0.360572	0.035773
C	2.314641	-0.667113	-0.066766
C	1.347172	0.419862	-0.543108
H	-2.454249	-0.785833	-0.753594
H	-1.957187	1.441667	-0.180564
H	-1.124523	0.347650	1.941971
H	-0.896641	1.530666	-1.604635
H	-0.521915	2.473174	-0.148577
H	3.273300	-0.567647	-0.585793
H	2.513636	-0.595644	1.006618
H	1.927251	-1.669198	-0.272032
H	1.749226	1.408194	-0.294669
H	1.263891	0.383949	-1.635632
H	0.417019	1.216380	1.958405
H	0.398355	-0.557442	1.952663

(*t*-AmylOOH, conformer 7, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164476	E(Thermal)=	0.172579
E(QCISD(T))=	-347.079567	E(Empiric)=	-0.208384
DE(MP2)=	-0.459977	DE(HF)=	-0.036424
G4MP2(0 K)=	-347.619876	G4MP2 Energy=	-347.611773
G4MP2 Enthalpy=	-347.610902	G4MP2 Free Energy=	-347.649670

Cartesian coordinates:

O	2.053344	-0.971652	0.020117
O	1.398377	0.182025	-0.554594
C	-2.273775	-0.785460	0.025377
C	-0.804384	-0.853916	-0.401588
C	-0.384101	1.643926	-0.680641
C	0.157671	0.535391	1.521296
C	0.062006	0.350933	0.006415
H	-2.804766	-1.679637	-0.316527
H	-2.784313	0.083262	-0.401740
H	-2.379901	-0.737372	1.113529
H	-1.372737	1.938581	-0.321212
H	-0.817048	0.802232	1.938072
H	-0.744407	-0.949890	-1.492576
H	-0.434537	1.514016	-1.765844
H	-0.353681	-1.757623	0.022381
H	1.859875	-1.657924	-0.637004
H	0.860084	1.340297	1.758822
H	0.499015	-0.380206	2.010434
H	0.314142	2.456037	-0.457676

(*t*-AmylOOH, conformer 8, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164117	E(Thermal)=	0.172366
E(QCISD(T))=	-347.076971	E(Empiric)=	-0.208384
DE(MP2)=	-0.459679	DE(HF)=	-0.036445
G4MP2(0 K)=	-347.617362	G4MP2 Energy=	-347.609113
G4MP2 Enthalpy=	-347.608242	G4MP2 Free Energy=	-347.647589

Cartesian coordinates:

O	-0.614784	1.050925	-0.616702
O	0.465344	1.933719	-0.236626
C	-1.786201	-0.924367	-0.456408
C	-0.500431	-0.099043	1.545187
C	-0.494093	-0.252025	0.024604
C	2.111374	-0.677864	0.015448
C	0.719511	-1.040166	-0.512994
H	-2.660746	-0.335086	-0.166602
H	-1.873161	-1.916495	-0.006146
H	-1.786262	-1.038526	-1.544684
H	-1.421638	0.392077	1.874236
H	-0.448152	-1.083404	2.020074
H	2.857296	-1.348262	-0.424950
H	2.393081	0.347050	-0.233108
H	2.174603	-0.791087	1.102315
H	0.703775	-0.950579	-1.605762
H	0.529975	-2.097225	-0.289958
H	0.349843	0.489030	1.896907
H	0.075942	2.416146	0.509277

(*t*-AmylOOH, conformer 9, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.164497	E(Thermal)=	0.172571
E(QCISD(T))=	-347.077165	E(Empiric)=	-0.208384
DE(MP2)=	-0.459621	DE(HF)=	-0.036445
G4MP2(0 K)=	-347.617118	G4MP2 Energy=	-347.609043
G4MP2 Enthalpy=	-347.608172	G4MP2 Free Energy=	-347.646971

Cartesian coordinates:

O	-0.624962	1.142591	-0.468059
O	0.481730	1.956844	-0.014317
C	-1.817557	-0.823394	-0.524676
C	-0.512915	-0.225822	0.017540
C	-0.506112	-0.242836	1.545602
C	2.073733	-0.768720	0.010206
C	0.688450	-0.961754	-0.617367
H	-2.679147	-0.239213	-0.189048
H	-1.930860	-1.847012	-0.158605
H	-1.814241	-0.845628	-1.618674
H	-1.424463	0.209312	1.932725
H	-0.450466	-1.273218	1.909940
H	2.809281	-1.372897	-0.531563
H	2.409027	0.270398	-0.022560
H	2.092451	-1.093634	1.055105
H	1.068487	1.937144	-0.785849
H	0.715688	-0.680213	-1.677046
H	0.450378	-2.031825	-0.593146
H	0.346123	0.306465	1.949903

(HMHP, conformer 1, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.060083	E(Thermal)=	0.064453
E(QCISD(T))=	-265.389074	E(Empiric)=	-0.123136
DE(MP2)=	-0.338578	DE(HF)=	-0.028917
G4MP2(0 K)=	-265.819623	G4MP2 Energy=	-265.815253
G4MP2 Enthalpy=	-265.814382	G4MP2 Free Energy=	-265.844274

Cartesian coordinates:

O	-1.404017	-0.533480	-0.188656
O	1.441421	-0.445422	0.189773
O	0.632997	0.626096	-0.348550
C	-0.639389	0.550517	0.267414
H	-1.130748	1.473004	-0.056973
H	-1.127195	-1.315273	0.305511
H	-0.516899	0.529596	1.355704
H	1.247966	-1.167974	-0.429262

(HMHP, conformer 2, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.060094 E(Thermal)=                  0.064440
 E(QCISD(T))=             -265.389399 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.338054 DE(HF)=                     -0.028928
 G4MP2(0 K)=              -265.819422 G4MP2 Energy=             -265.815076
 G4MP2 Enthalpy=          -265.814205 G4MP2 Free Energy=        -265.844067
Cartesian coordinates:
O         -1.351455   -0.608075   -0.014839
O          1.463418   -0.437088    0.177768
O          0.625090    0.596716   -0.385733
C         -0.624088    0.555224    0.276765
H         -1.642038   -0.551177   -0.934645
H         -1.121018    1.467080   -0.076514
H         -0.477666    0.577262    1.360022
H          1.088828   -1.236929   -0.227020
```

(HMHP, conformer 3, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.059860 E(Thermal)=                  0.064323
 E(QCISD(T))=             -265.388305 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.338690 DE(HF)=                     -0.028960
 G4MP2(0 K)=              -265.819230 G4MP2 Energy=             -265.814767
 G4MP2 Enthalpy=          -265.813896 G4MP2 Free Energy=        -265.844040
Cartesian coordinates:
O         -1.458642   -0.494886   -0.179761
O          1.404345   -0.547288    0.031068
O          0.617868    0.597101   -0.376374
C         -0.624024    0.523937    0.299631
H         -1.155659   -1.325197    0.208510
H         -1.095788    1.482765    0.062544
H         -0.445025    0.430707    1.377097
H          1.932046   -0.171312    0.754595
```

(HMHP, conformer 4, PG = C_1, NImag = 0)

```
Thermochemistry:
 Temperature=              275.150000 Pressure=                    1.000000
 E(ZPE)=                     0.059991 E(Thermal)=                  0.064381
 E(QCISD(T))=             -265.388393 E(Empiric)=                 -0.123136
 DE(MP2)=                   -0.338414 DE(HF)=                     -0.028998
 G4MP2(0 K)=              -265.818950 G4MP2 Energy=             -265.814560
 G4MP2 Enthalpy=          -265.813689 G4MP2 Free Energy=        -265.843621
Cartesian coordinates:
O         -1.423184   -0.579038   -0.012210
O          1.432297   -0.540057    0.054072
O          0.604622    0.551314   -0.414570
C         -0.614183    0.520821    0.302421
H         -1.746508   -0.457410   -0.914353
H         -1.077185    1.476777    0.026025
H         -0.417524    0.477582    1.377378
H          2.016438   -0.079628    0.678087
```

(HMHP, conformer 5, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.059253	E(Thermal)=	0.063868
E(QCISD(T))=	-265.383330	E(Empiric)=	-0.123136
DE(MP2)=	-0.339127	DE(HF)=	-0.029010
G4MP2(0 K)=	-265.815351	G4MP2 Energy=	-265.810736
G4MP2 Enthalpy=	-265.809865	G4MP2 Free Energy=	-265.840270

Cartesian coordinates:

O	-1.752221	0.065591	0.151310
O	-0.472791	-0.549661	-0.094439
O	1.755354	-0.127126	-0.091695
C	0.512146	0.491968	0.019915
H	-2.032982	0.310100	-0.745503
H	1.941535	-0.573174	0.744793
H	0.406510	1.192180	-0.816429
H	0.369324	1.008655	0.976243

(HMHP, conformer 6, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.059294	E(Thermal)=	0.063882
E(QCISD(T))=	-265.383266	E(Empiric)=	-0.123136
DE(MP2)=	-0.339166	DE(HF)=	-0.029018
G4MP2(0 K)=	-265.815292	G4MP2 Energy=	-265.810704
G4MP2 Enthalpy=	-265.809833	G4MP2 Free Energy=	-265.840144

Cartesian coordinates:

O	-1.755568	-0.134919	-0.060478
O	1.759462	0.095841	-0.057056
O	0.473662	-0.553087	-0.088245
C	-0.511991	0.491538	-0.012811
H	-1.927249	-0.524588	0.806583
H	-0.423702	1.142567	-0.888471
H	-0.352889	1.062708	0.910909
H	1.955340	0.107401	0.894083

(DSS, conformer 1, PG = C_s, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.204406	E(Thermal)=	0.218131
E(QCISD(T))=	-1148.777463	E(Empiric)=	-0.322048
DE(MP2)=	-0.827980	DE(HF)=	-0.067724
G4MP2(0 K)=	-1149.790809	G4MP2 Energy=	-1149.777085
G4MP2 Enthalpy=	-1149.776213	G4MP2 Free Energy=	-1149.830112

Cartesian coordinates:

S	0.169617	-2.929201	-0.000000
Si	-0.095464	2.762614	0.000000
O	-0.764637	-4.069258	-0.000000
O	0.984566	-2.856275	-1.227628
O	0.984566	-2.856275	1.227628
C	-1.388661	4.134633	-0.000000
C	-0.988729	1.091465	-0.000000
C	-0.870735	-1.456081	-0.000000
C	-0.077182	-0.148231	-0.000000
C	0.984566	2.913987	-1.538868
C	0.984566	2.913987	1.538868
H	-2.034285	4.075666	-0.883877
H	-2.034285	4.075666	0.883877
H	-1.653262	1.057114	-0.875075
H	-1.653262	1.057114	0.875075
H	-1.509914	-1.532465	-0.885388
H	-1.509914	-1.532465	0.885388
H	-0.920406	5.125764	-0.000000
H	1.768266	2.148423	-1.559733
H	1.768266	2.148423	1.559733
H	1.480458	3.890795	-1.580417
H	1.480458	3.890795	1.580417
H	0.577452	-0.135344	-0.878643
H	0.577452	-0.135344	0.878643
H	0.393347	2.806193	-2.455620
H	0.393347	2.806193	2.455620

(DSS, conformer 2, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.204699	E(Thermal)=	0.218267
E(QCISD(T))=	-1148.775626	E(Empiric)=	-0.322048
DE(MP2)=	-0.828306	DE(HF)=	-0.067677
G4MP2(0 K)=	-1149.788958	G4MP2 Energy=	-1149.775390
G4MP2 Enthalpy=	-1149.774519	G4MP2 Free Energy=	-1149.828335

Cartesian coordinates:

S	-2.710057	0.092577	0.027041
Si	2.529351	0.076103	0.009933
O	-3.315974	-1.132088	-0.528202
O	-3.303316	1.324448	-0.522937
O	-2.664803	0.087186	1.501895
C	-0.993977	0.104147	-0.527531
C	-0.198037	-1.112250	-0.053396
C	4.212977	-0.526170	-0.591607
C	2.509670	0.121785	1.895362
C	2.244295	1.817860	-0.659339
C	1.237498	-1.168321	-0.614175
H	-1.028503	0.153051	-1.620631
H	-0.743266	-2.013009	-0.358262
H	-0.570426	1.043339	-0.162098
H	-0.177306	-1.119009	1.042089
H	5.016546	0.145470	-0.267912
H	4.443133	-1.526409	-0.207089
H	4.250144	-0.578358	-1.686097
H	3.299966	0.775456	2.282680
H	3.096991	2.465047	-0.420794
H	2.668068	-0.874702	2.323671
H	2.129620	1.816478	-1.749393
H	1.652924	-2.160346	-0.385933
H	1.555967	0.499170	2.281109
H	1.350944	2.286444	-0.233212
H	1.203396	-1.117973	-1.711772

(DSS, conformer 3, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.204608	E(Thermal)=	0.218189
E(QCISD(T))=	-1148.775539	E(Empiric)=	-0.322048
DE(MP2)=	-0.827557	DE(HF)=	-0.067691
G4MP2(0 K)=	-1149.788226	G4MP2 Energy=	-1149.774645
G4MP2 Enthalpy=	-1149.773774	G4MP2 Free Energy=	-1149.827376

Cartesian coordinates:

S	2.680753	-0.171671	0.015855
Si	-2.541984	-0.089120	-0.009164
O	3.997871	0.236978	-0.504807
O	2.642209	-0.238847	1.489515
O	2.178659	-1.403184	-0.622963
C	-3.477283	-1.306260	-1.104648
C	-3.399080	1.590787	-0.065209
C	-2.530619	-0.723946	1.767364
C	-0.768248	0.057486	-0.653823
C	1.565668	1.173721	-0.445272
C	0.132179	1.057709	0.091379
H	-4.512249	-1.435295	-0.767266
H	-4.443350	1.513654	0.259600
H	-3.549896	-0.856949	2.148461
H	-3.510588	-0.963413	-2.145301
H	-3.400526	2.006181	-1.079677
H	-3.003570	-2.294764	-1.099173
H	-2.906858	2.319238	0.588891
H	-2.022581	-1.692408	1.842250
H	-2.017289	-0.029768	2.442274
H	-0.811923	0.334971	-1.717070
H	-0.313778	-0.939400	-0.628577
H	-0.311843	2.058866	0.031971
H	2.049593	2.074158	-0.054684
H	1.582842	1.231346	-1.538230
H	0.182115	0.811438	1.158447

(DSS, conformer 4, PG = C_1, NImag = 0)

Thermochemistry:

Temperature=	275.150000	Pressure=	1.000000
E(ZPE)=	0.205077	E(Thermal)=	0.218389
E(QCISD(T))=	-1148.774858	E(Empiric)=	-0.322048
DE(MP2)=	-0.827277	DE(HF)=	-0.067587
G4MP2(0 K)=	-1149.786693	G4MP2 Energy=	-1149.773381
G4MP2 Enthalpy=	-1149.772509	G4MP2 Free Energy=	-1149.825268

Cartesian coordinates:

S	2.372645	-0.198382	-0.039419
Si	-2.232004	-0.119884	0.003082
O	3.290655	-0.614636	1.035898
O	3.025218	0.641706	-1.060509
O	1.638363	-1.338030	-0.626209
C	-3.344515	-0.902203	-1.305051
C	-3.224120	1.133187	1.006233
C	-1.614876	-1.481843	1.157100
C	-0.833964	0.763927	-0.927242
C	1.155764	0.858450	0.779744
C	0.191552	1.609592	-0.146435
H	-4.198880	-1.415266	-0.848452
H	-4.074094	0.655268	1.507417
H	-3.741622	-0.151961	-1.998496
H	-3.623699	1.931813	0.370548
H	-2.797531	-1.642628	-1.900571
H	-2.611676	1.605099	1.783048
H	-2.441558	-2.138616	1.453475
H	-1.342654	1.431567	-1.637916
H	-1.179179	-1.074921	2.076126
H	-0.851261	-2.102960	0.677340
H	-0.338279	2.342424	0.475001
H	-0.312415	0.025661	-1.546241
H	1.753435	1.575951	1.349930
H	0.796468	2.193819	-0.850155
H	0.635749	0.218265	1.496969

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(2) Milas, N. A.; Surgenor, D. M. Studies in Organic Peroxides. X. t-Amyl Hydroperoxide and Di-t-amyl Peroxide. *J. Am. Chem. Soc.* **1946**, *68*, 643-644.