Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for:

Stereo-Electronic Factors Influencing the Stability of Hydroperoxyalkyl Radicals: Transferability of Chemical Trends across Hydrocarbons and *ab initio* Methods

Saurabh Chandra Kandpal,[†] Kgalaletso P. Otukile,[‡] Shweta Jindal,[†] Salini Senthil,[†] Cameron Matthews,[‡] Sabyasachi Chakraborty,[†] Lyudmila V. Moskaleva,[*,‡] and Raghunathan Ramakrishnan[*,†]

[†]*Tata Institute of Fundamental Research, Hyderabad 500046, India*

[‡]*Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein 9300, South Africa*

E-mail: moskaleval@ufs.ac.za; ramakrishnan@tifrh.res.in

Table of Contents

DFT Benchmarking

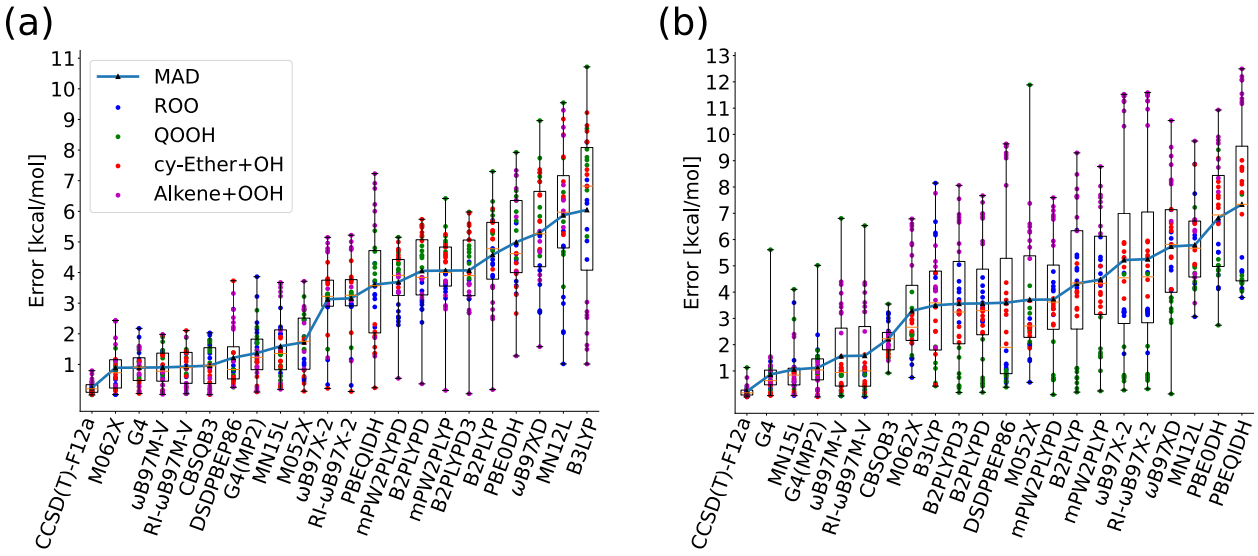

Figure S1: Ranking of the prediction accuracy of DFAs and cWFTs for reaction barriers using box-and-whisker plot. For a given method, the Box-and-whisker plot depicts the deviation in energy with respect to W1 energy of (a) Reaction species and (b) Reaction barriers for all the benchmark systems. For boxplots, the centre line denotes the median, the box displays the interquartile range, and the whiskers indicate the range. The MAD for each method is connected by blue line. Methods are sorted in ascending order of MAD. RI-ωB97M-V and RI-ωB97X-2 represent the methods where RI approximation was activated.

Table S1: ΔU^{ROO} and ΔU^{TS4} energies (with respect to R· + O_2) for dataset systems calculated with W1, CCSD(T)-F12a/cc-pVDZ-F12, G4, and RI-ωB97M-V methods. In the table, CC and DFT represent CCSD(T)-F12a/cc-pVDZ-F12 and RI-ωB97M-V, respectively.

Species	$\Delta U^{\mathrm{ROO}}_{\mathrm{W1}}$	$\Delta U^{\mathrm{ROO}}_{\mathrm{CC}}$	$\Delta U^{\mathrm{ROO}}_{\mathrm{G4}}$	$\Delta U^{\mathrm{ROO}}_{\mathrm{DFT}}$	$\Delta U^{\mathrm{TS4}}_{\mathrm{W1}}$	$\Delta U^{\mathrm{TS4}}_{\mathrm{CC}}$	$\Delta U^{\mathrm{TS4}}_{\mathrm{G4}}$	$\Delta U^{\mathrm{TS4}}_{\mathrm{DFT}}$
Ethyl	-32.82	-33.03	-33.45	-34.23	-1.52	-1.70	-0.30	2.08
Isopropyl	-34.58	-34.75	-35.74	-35.55	-4.94	-5.06	-3.97	-0.46
Isobutyl	-33.66	-33.70	-34.53	-35.01	-11.99	-11.90	-10.44	-9.48
Tertbutyl	-36.65	-35.94	-37.20	-36.24	-6.74	-7.18	-6.25	-2.37
Neopentyl	-33.73	-33.74	-34.67	-35.13	0.71	0.47	2.20	3.96
cy-hexyl	-33.45	-35.58	-36.83	-36.36	-8.55	-8.71	-7.54	-5.10
cy-hexenyl	-19.63	-19.84	-21.52	-20.29	7.29	7.07	7.91	11.28
cy-hexadienyl	-11.13	-11.50	-13.31	-11.21	3.67	2.92	4.89	6.92

Table S2: Comparison of performance of CCSD(T)-F12a/cc-pVDZ-F12, G4 and RI-ωB97M-V with respect to W1 for ROO· and TS4. Here, $\Delta\Delta U^{\mathrm{ROO}}_{1} = \Delta U^{\mathrm{W1}}_{\mathrm{ROO}}$- $\Delta U^{\mathrm{CC}}_{\mathrm{ROO}}$, $\Delta\Delta U^{\mathrm{ROO}}_{2} = \Delta U^{\mathrm{W1}}_{\mathrm{ROO}}$- $\Delta U^{\mathrm{G4}}_{\mathrm{ROO}}$, $\Delta\Delta U^{\mathrm{ROO}}_{3} = \Delta U^{\mathrm{W1}}_{\mathrm{ROO}}$- $\Delta U^{\mathrm{RI}}_{\mathrm{ROO}}$, $\Delta\Delta U^{\mathrm{TS4}}_{1} = \Delta U^{\mathrm{W1}}_{\mathrm{TS4}}$- $\Delta U^{\mathrm{CC}}_{\mathrm{TS4}}$, $\Delta\Delta U^{\mathrm{TS4}}_{2} = \Delta U^{\mathrm{W1}}_{\mathrm{TS4}}$- $\Delta U^{\mathrm{G4}}_{\mathrm{TS4}}$, and $\Delta\Delta U^{\mathrm{TS4}}_{3} = \Delta U^{\mathrm{W1}}_{\mathrm{TS4}}$- $\Delta U^{\mathrm{RI}}_{\mathrm{TS4}}$.

Species	$\Delta\Delta U^{\mathrm{ROO}}_{1}$	$\Delta\Delta U^{\mathrm{ROO}}_{2}$	$\Delta\Delta U^{\mathrm{ROO}}_{3}$	$\Delta\Delta U^{\mathrm{TS4}}_{1}$	$\Delta\Delta U^{\mathrm{TS4}}_{2}$	$\Delta\Delta U^{\mathrm{TS4}}_{3}$
Ethyl	0.21	0.63	1.41	0.18	-1.18	-3.60
Isopropyl	0.17	1.16	0.97	0.32	-0.77	-4.28
Isobutyl	0.04	0.87	1.35	-0.09	-1.55	-2.51
Tertbutyl	0.29	1.55	0.59	0.44	-0.49	-4.27
Neopentyl	0.01	0.94	1.40	0.24	-1.49	-3.25
cy-hexyl	0.13	1.38	0.91	0.16	-1.01	-3.45
cy-hexenyl	0.21	1.89	0.66	0.22	-0.62	-3.99
cy-hexadienyl	0.37	2.18	0.08	0.75	-1.22	-3.25

Spin contamination

Based on the results presented in Table. IV in the main text, it is evident that the MAD is highest for TS4 for all the density functional theory (DFT) functionals considered, except for MN15L. This significant deviation for TS4 is the primary contributor to the considerably high MAD values observed for energy barriers for all the functionals. To understand the cause of this high deviation for TS4, the $< S^2 >$ values for all reaction species and functionals were examined. The ideal value of $< S^2 >$ for a singlet radical is 0.75. When $< S^2 >$ deviates from this value, it is known as spin-contamination or spin error. The higher the deviation, the higher the spin contamination. The results in FigureS3 demonstrate that the spin mean absolute error (MAE) for TS4 is higher than that for the other reaction species. The Pearson's correlation coefficient between spin MAE and energy MAE is 0.81 for TS4, indicating that the higher energy MAE of TS4 is due to its higher spin MAE. Furthermore, the $< S^2 >$ values for TS4 exhibit a more significant deviation from the ideal value compared to the other TS. While TS1, TS2, and TS3 have all their data points between 0.75 and 1.0, TS4 has $< S^2 >$ values higher than 1.0 for many functionals, which indicates higher spin contamination for TS4. The higher the spin contamination for TS4, the higher the MAD for all the functionals. Hence, this high spin contamination for TS4 may be one of the main reasons for the very high MAD values.

When different functionals were compared, MN15L was found to be the best-performing functional for TS, showing very low spin contamination for all the TS. In this study, all the Minnesota functionals (M06-2X, M05-2X, MN15L, MN12L) exhibited very low spin contamination compared to other functionals. Additionally, ωB97M-V also had low spin contamination and low MAD for TS4. However, DSDPBEP86, ωB97X-2, and PBEQIDH exhibited high spin contamination for TS4 and very high MAD values of 9.25 kcal/mol, 11.21, and 11.77 kcal/mol, respectively.

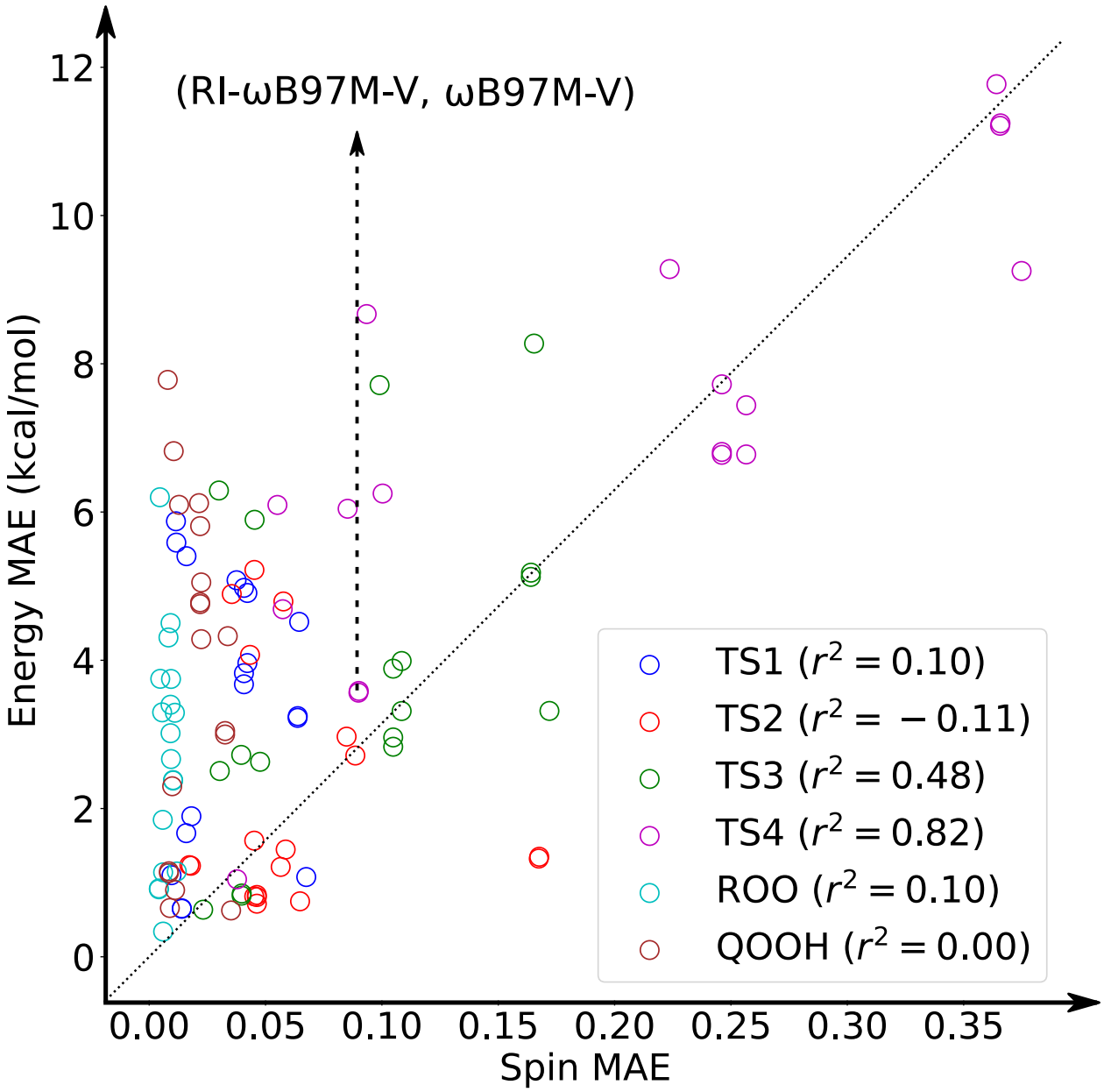

Figure S2: Scatter plot between energy mean absolute error (Energy MAE) and spin mean absolute error (Spin MAE) for reaction species. Each point in the plot represents a DFT functional for the given species. Values in the parenthesis are Pearson's correlation coefficient.

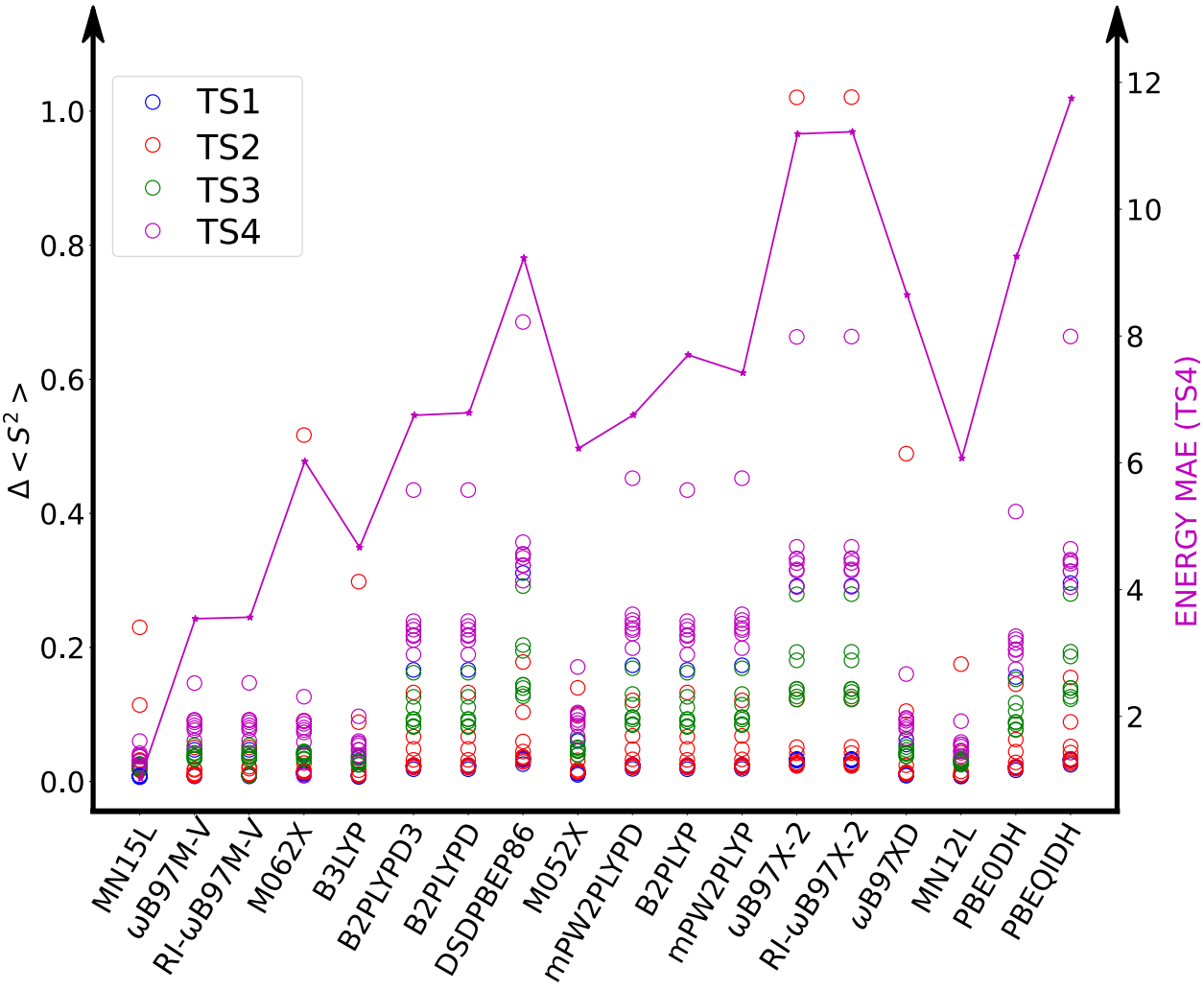

Figure S3: Scatter plot showing the difference between ideal and calculated $< S^2 >$ values of TS of all systems for all DFT functionals. The left-hand side y-axis represents $\Delta < S^2 >$ values. The solid pink line and the right-hand side y-axis represent the MAD for TS4. Methods are sorted in ascending order of MAD for TS.

Low-temperature hydrocarbon combustion mechanism and the associated reactive intermediates for R·

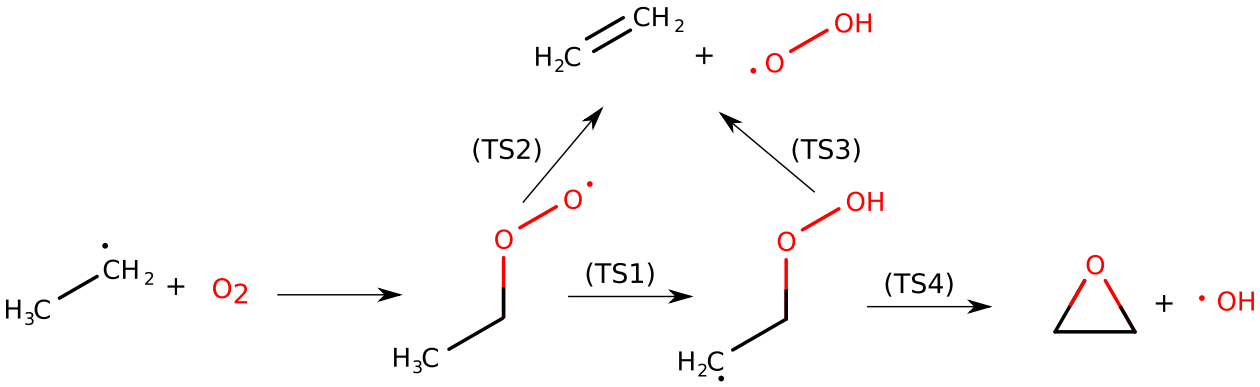

Figure S4: The reactive intermediates for ethyl radical combustion

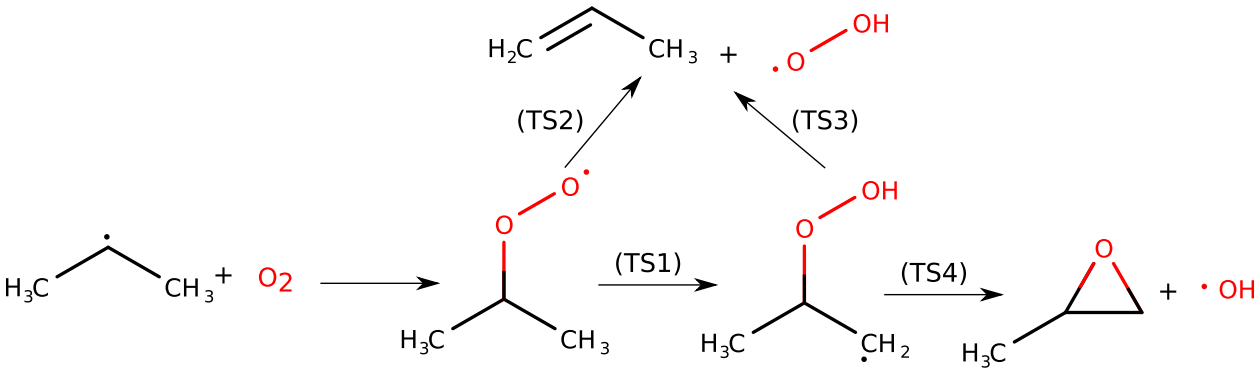

Figure S5: The reactive intermediates for isopropyl radical combustion

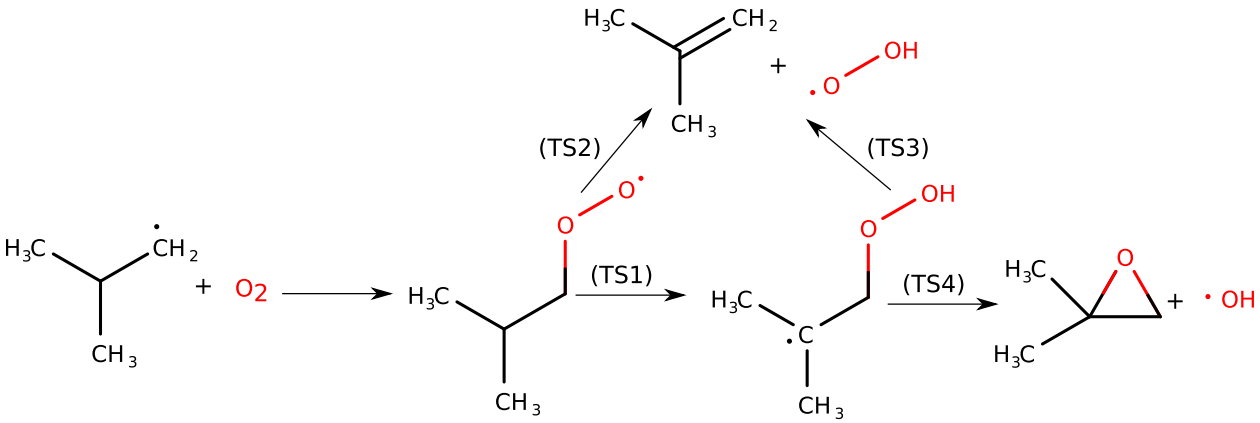

Figure S6: The reactive intermediates for isobutyl radical combustion

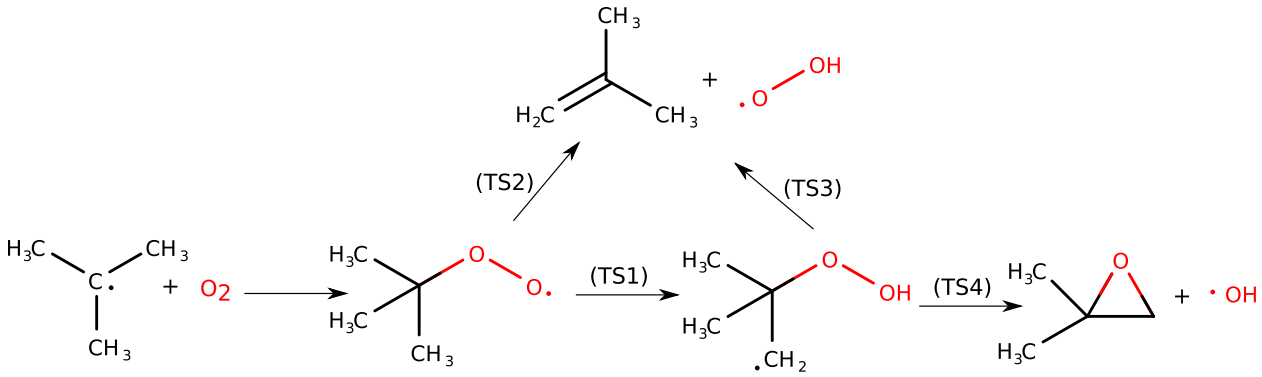

Figure S7: The reactive intermediates for tertbutyl radical combustion

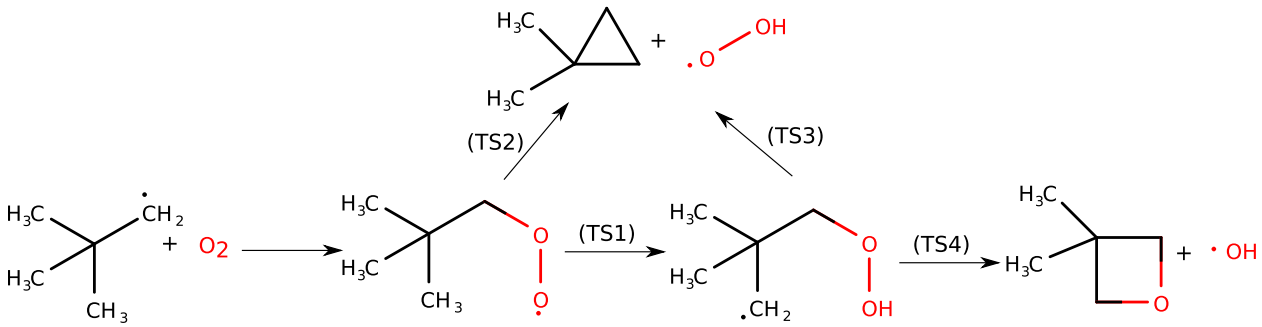

Figure S8: The reactive intermediates for neopentyl radical combustion

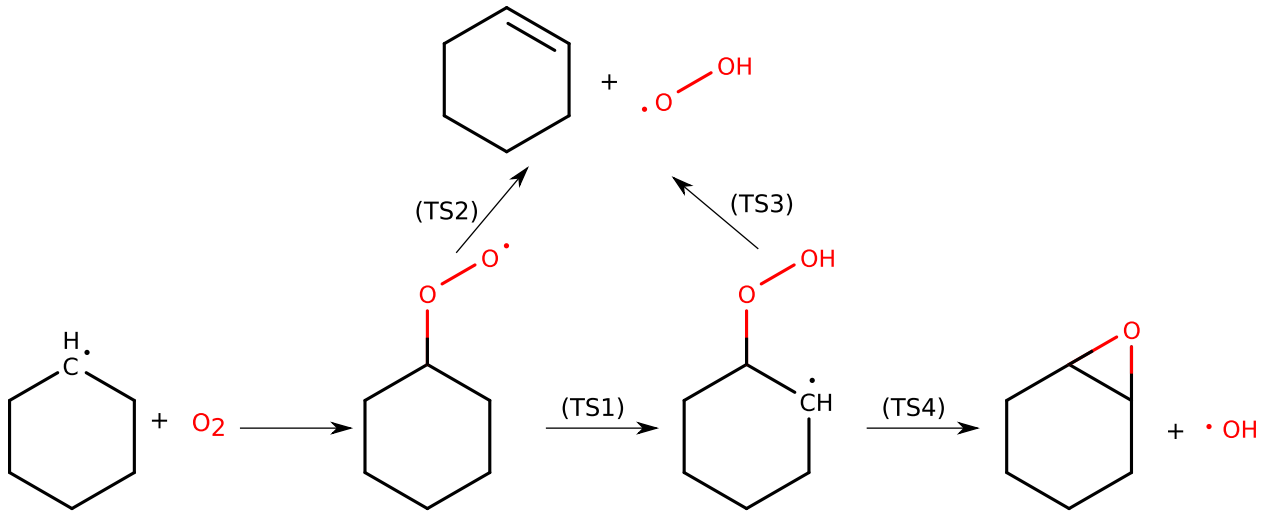

Figure S9: The reactive intermediates for cyclohexyl radical combustion

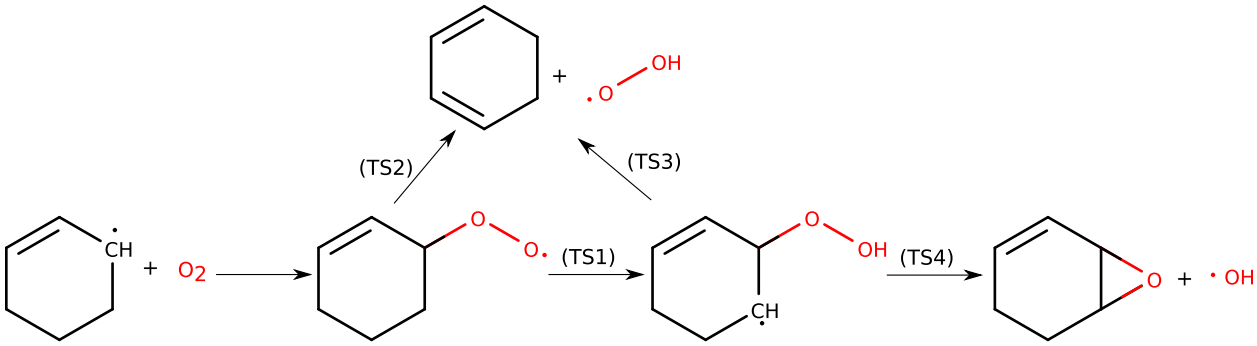

Figure S10: The reactive intermediates for α-cyclohexenyl radical combustion

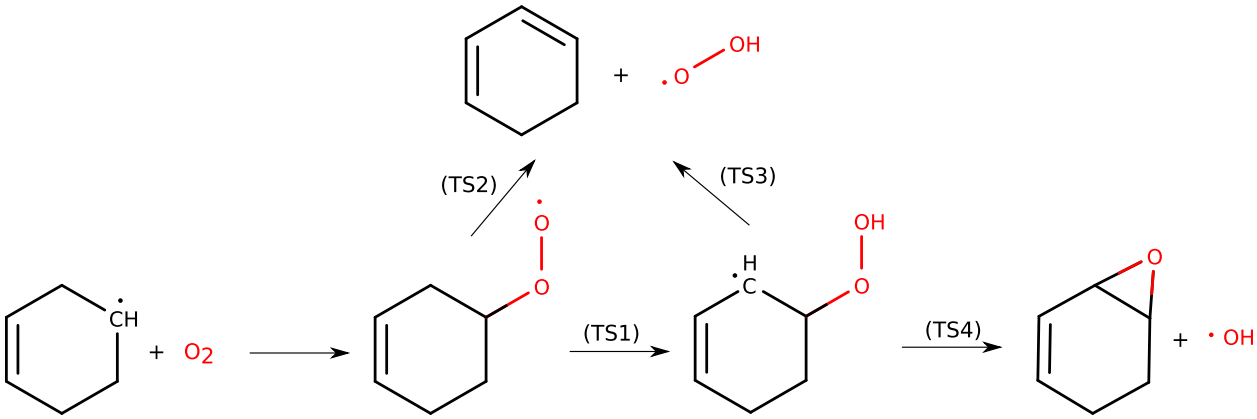

Figure S11: The reactive intermediates for β-cyclohexenyl radical combustion

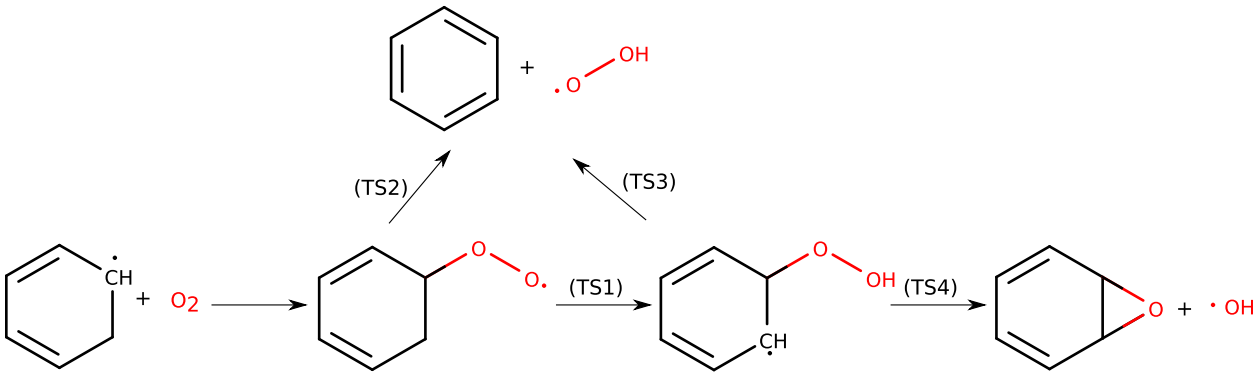

Figure S12: The reactive intermediates for cyclohexadienyl radical combustion

IRC Profiles for the different reactions in low-temperature combustion

The IRC profiles are represented in the following order for all the hydrocarbons

a) ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

b) ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

c) ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

d) ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

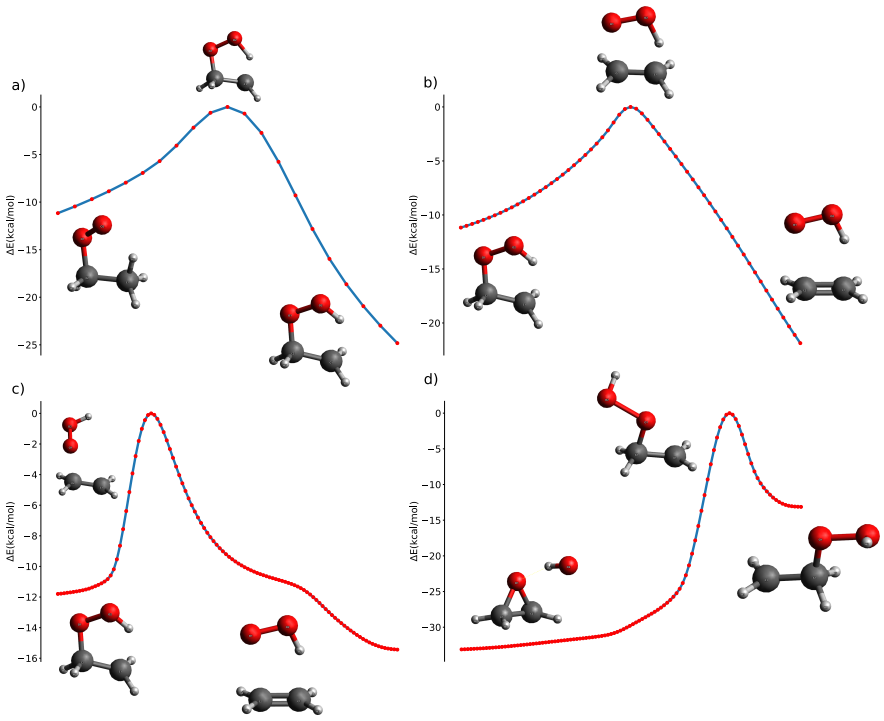

Figure S13: The IRC profile for the combustion of ethyl radical

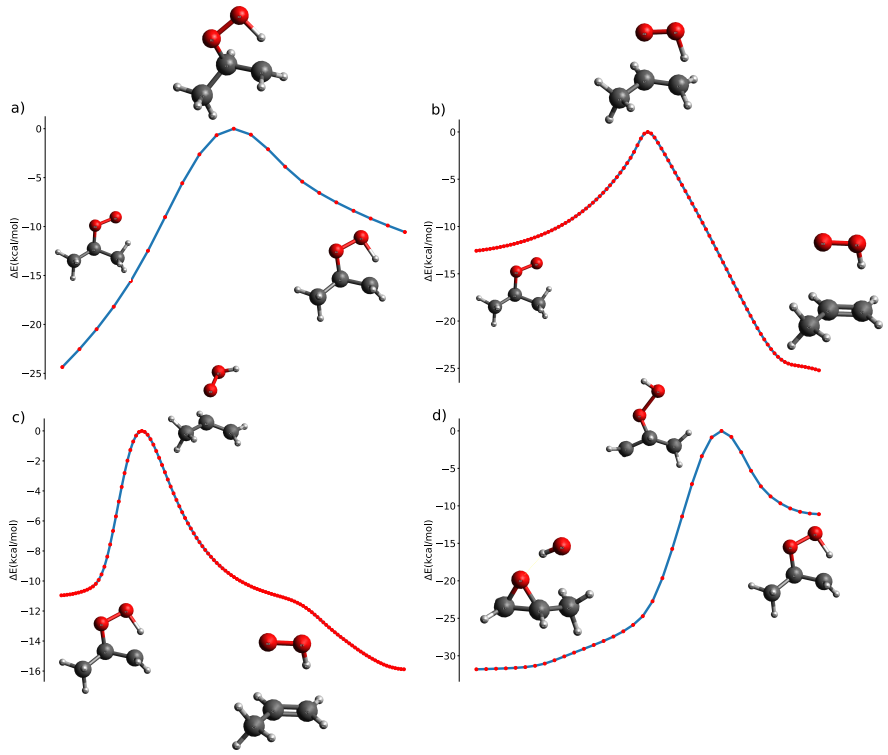

Figure S14: The IRC profile for the combustion of isopropyl radical

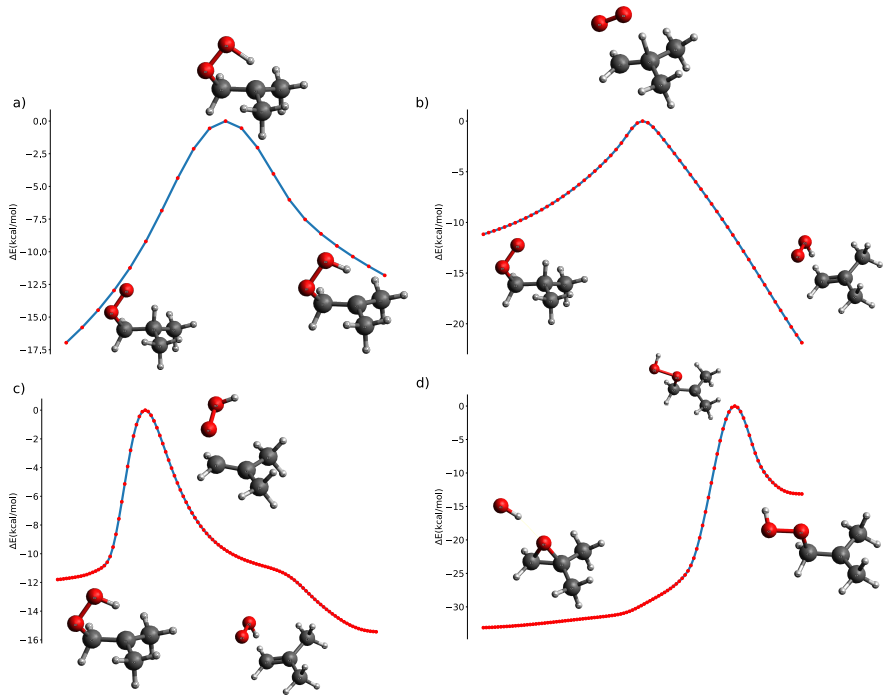

Figure S15: The IRC profile for the combustion of isobutyl radical

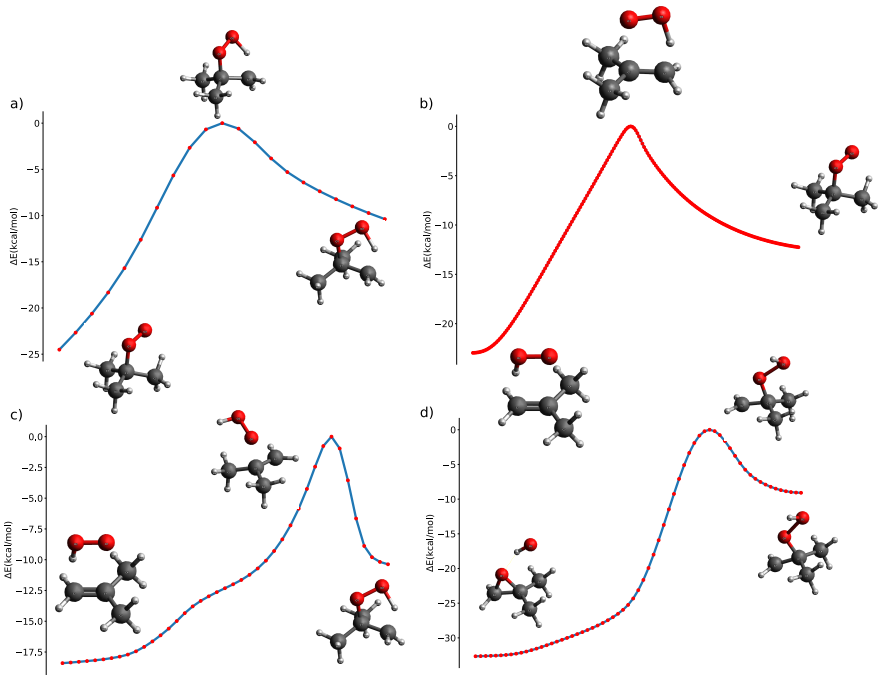

Figure S16: The IRC profile for the combustion of tertbutyl radical

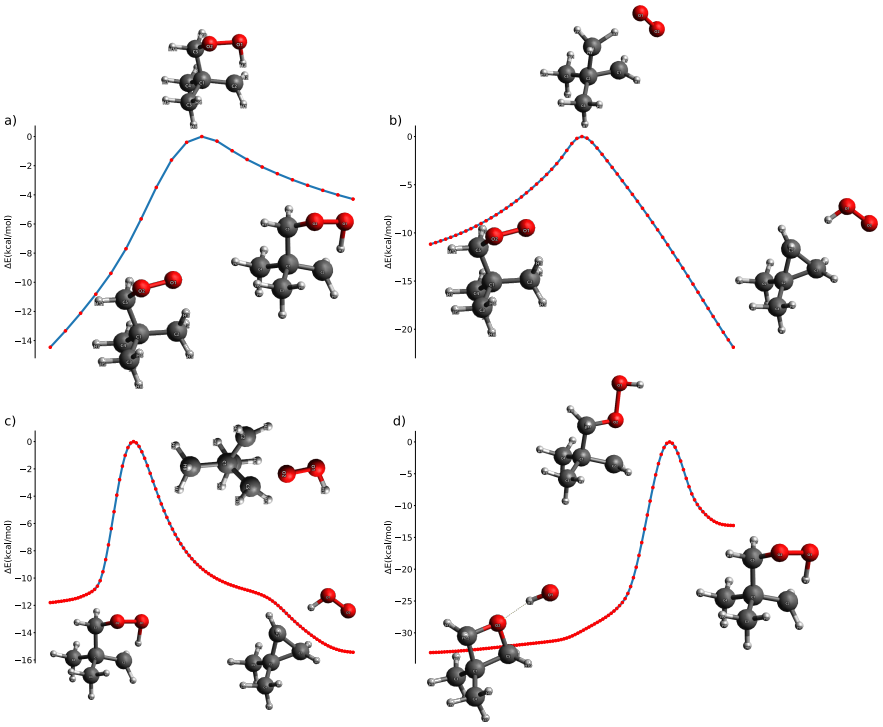

Figure S17: The IRC profile for the combustion of neopentyl radical

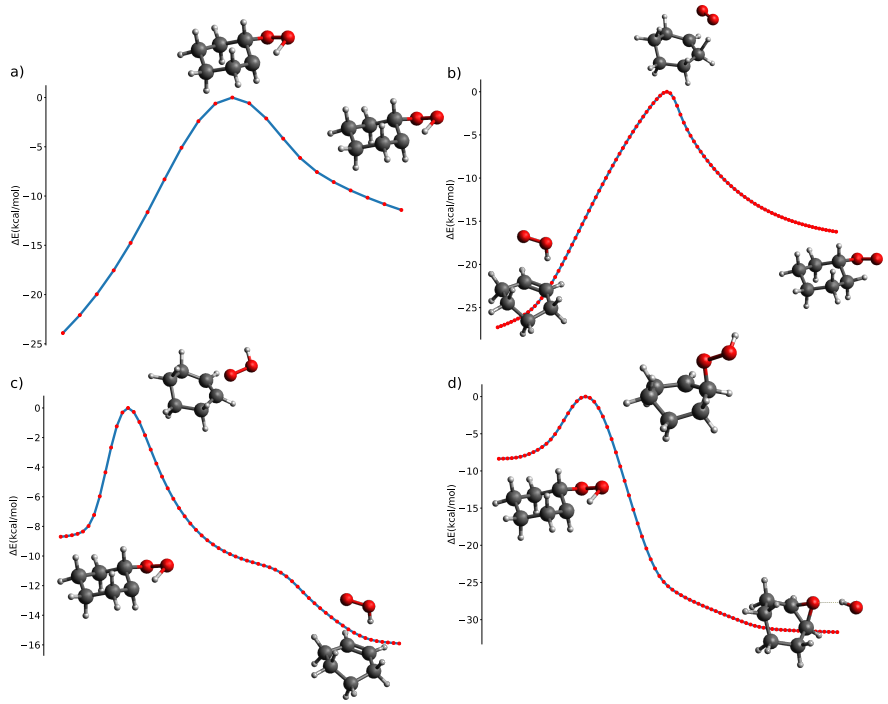

Figure S18: The IRC profile for the combustion of cyclohexyl radical

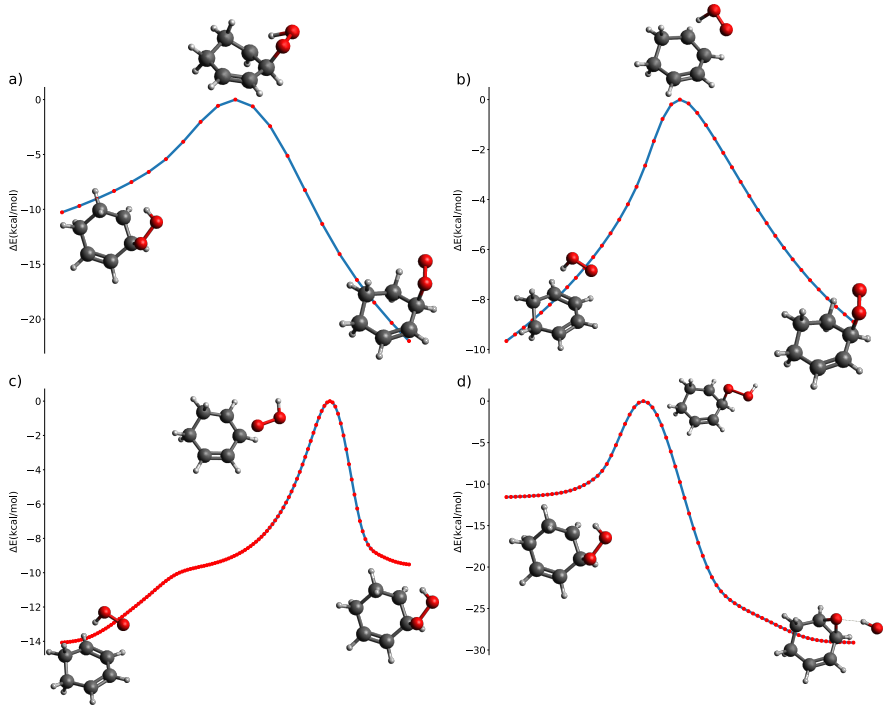

Figure S19: The IRC profile for the combustion of α-cyclohexenyl radical

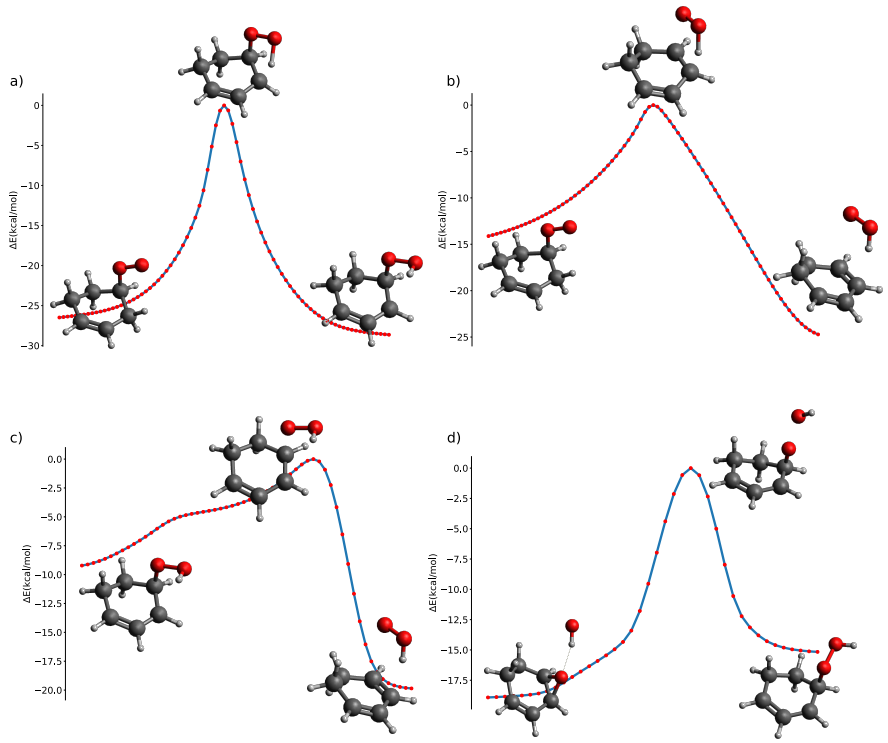

Figure S20: The IRC profile for the combustion of β-cyclohexenyl radical

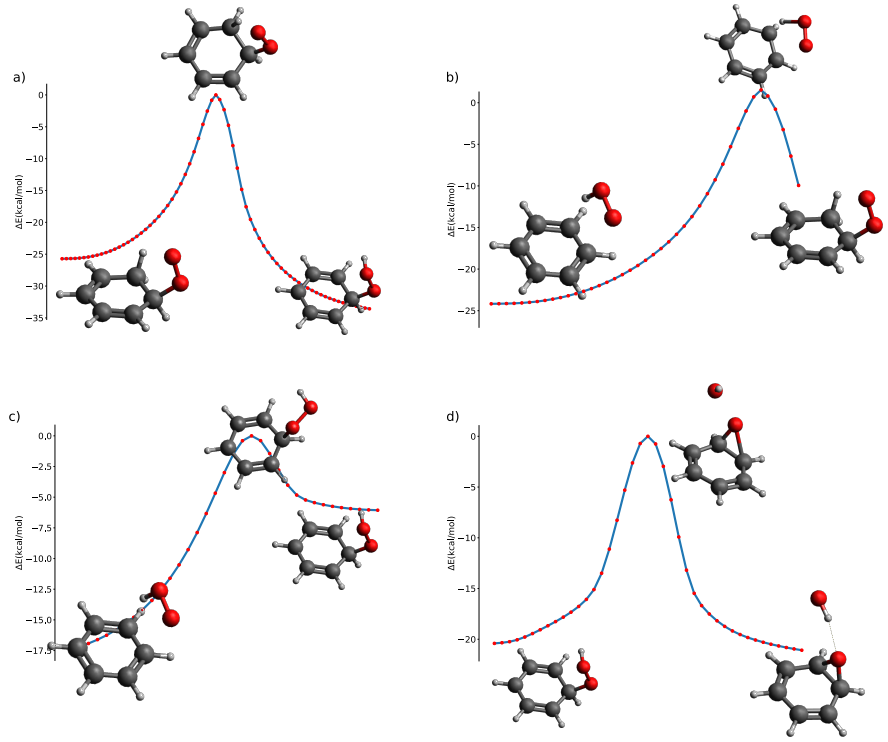

Figure S21: The IRC profile for the combustion of cyclohexadienyl radical

W1-level equilibrium geometry, harmonic frequencies, and thermochemistry energies of different reaction species involved in combustion reaction of R·

Hydrocarbon 1: ethyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.691636   -0.000000   -0.002049
C    -0.792081    0.000000   -0.017585
H     1.103759   -0.884476   -0.491892
H     1.091851    0.000004    1.022920
H     1.103759    0.884472   -0.491898
H    -1.348350   -0.924419    0.039336
H    -1.348349    0.924419    0.039336

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    104.8073    486.2223    813.8449    982.2743   1061.8581   1195.8772   1402.1395
   1467.3672   1481.5538   1482.2557   2943.0673   3034.7866   3077.3432   3142.6027
   3240.6016


== Thermochemistry energies (hartree) ==
  ZPVE =     0.058156  (after scaling by 0.985)
W1  Ee =  -79.168722  (total electronic energy)
W1  U0 =  -79.110566  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -79.029415  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.744457   -0.181342   -0.000005
C     0.414201    0.535217    0.000005
H     1.852261   -0.807843    0.884837
H     2.551771    0.551299   -0.000002
H     1.852256   -0.807830   -0.884857
O    -0.633958   -0.480438    0.000009
H     0.265409    1.148873    0.887848
H     0.265397    1.148879   -0.887833
O    -1.833422    0.060860   -0.000007

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     74.2528    223.5669    307.1919    502.3475    805.6244    841.9603   1015.2529
   1133.9237   1150.2037   1193.6478   1278.2306   1381.0735   1420.0700   1486.8332
   1496.2760   1508.8877   3043.2166   3055.1942   3096.0954   3109.4166   3120.8248



== Thermochemistry energies (hartree) ==
  ZPVE =     0.070111  (after scaling by 0.985)
W1  Ee =  -229.643821  (total electronic energy)
W1  U0 =  -229.573710  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.268433  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.852200   -0.166980    0.027775
C    -0.531369    0.493419    0.058741
H    -2.708700    0.334573   -0.394654
H    -1.980039   -1.139938    0.478434
O     0.457468   -0.513383   -0.173682
H    -0.450756    1.278182   -0.699368
H    -0.333842    0.959118    1.037207
O     1.752335    0.130903   -0.036404
H     2.096334   -0.330729    0.739984

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    110.0437    129.5381    203.3557    300.0234    469.0284    512.6005    819.4553
    933.8400    986.9561   1071.2743   1143.1600   1225.4651   1359.2805   1383.6467
   1454.7737   1496.5921   2921.5501   3022.7943   3156.2382   3264.6239   3758.8937



== Thermochemistry energies (hartree) ==
  ZPVE =     0.066698  (after scaling by 0.985)
W1  Ee =  -229.614038  (total electronic energy)
W1  U0 =  -229.547339  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.238190  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.731430   -0.371702    0.000000
C    -0.731430   -0.371702   -0.000000
O    -0.000000    0.853606   -0.000000
H     1.266004   -0.592106   -0.918210
H     1.266004   -0.592106    0.918209
H    -1.266003   -0.592106    0.918210
H    -1.266004   -0.592106   -0.918209

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    820.9816    846.5212    892.4287   1047.1821   1150.3912   1156.3546   1171.7311
   1177.3731   1301.7028   1507.0326   1541.1250   3078.8490   3085.5370   3157.5797
   3173.3447


== Thermochemistry energies (hartree) ==
  ZPVE =     0.056343  (after scaling by 0.985)
W1  Ee =  -153.855513  (total electronic energy)
W1  U0 =  -153.799170  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -153.598131  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.000000   -0.661966   -0.000000
C     0.000000    0.661966    0.000000
H    -0.920567   -1.231546    0.000000
H     0.920567   -1.231546   -0.000000
H    -0.920567    1.231546    0.000000
H     0.920567    1.231546   -0.000000

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    835.8298    978.9608    983.5714   1067.0956   1246.4512   1382.3409   1478.8937
   1693.3624   3126.1146   3139.9061   3195.1940   3223.6535


== Thermochemistry energies (hartree) ==
  ZPVE =     0.050156  (after scaling by 0.985)
W1  Ee =  -78.604857  (total electronic energy)
W1  U0 =  -78.554701  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -78.465674  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.222388   -0.566466   -0.119613
H    -1.941196   -0.966413    0.586382
H     0.022943   -1.137914    0.059018
H    -1.471076   -0.736313   -1.162951
C    -0.540324    0.752654    0.211403
H    -0.961280    1.623724   -0.293709
H    -0.528184    0.915931    1.291989
O     0.791214    0.598096   -0.290043
O     1.140669   -0.700114    0.161109

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2274.2560    274.9541    438.7388    554.4706    687.2618    868.9591    899.9893
    906.2836    962.5398   1047.0938   1110.8987   1169.2613   1244.6992   1346.9688
   1456.7294   1499.5115   1723.6265   3022.5170   3077.4755   3101.5997   3192.2292



== Thermochemistry energies (hartree) ==
  ZPVE =     0.064146  (after scaling by 0.985)
W1  Ee =  -229.578911  (total electronic energy)
W1  U0 =  -229.514765  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.203690  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.285569   -0.616825    0.000027
H    -1.630771   -1.085342    0.915429
H     0.026458   -0.950626   -0.000075
H    -1.630877   -1.085201   -0.915406
C    -1.044096    0.743790    0.000118
H    -1.023461    1.316997   -0.914815
H    -1.023353    1.316856    0.915137
O     1.145733    0.615227   -0.000019
O     1.261766   -0.649536   -0.000123

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1089.2415    216.0393    354.2849    478.9129    516.9775    643.5291    832.9459
    891.5177   1016.0131   1040.6236   1233.2915   1299.5412   1315.1097   1334.4709
   1474.4510   1571.0968   1599.0782   3102.4777   3160.7059   3177.7927   3246.4129



== Thermochemistry energies (hartree) ==
  ZPVE =     0.063966  (after scaling by 0.985)
W1  Ee =  -229.587475  (total electronic energy)
W1  U0 =  -229.523509  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.211904  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.625492    0.535263   -0.115726
H    -2.181955    0.478982   -1.040579
H     1.676417    1.144824   -0.288345
H    -1.556027    1.502362    0.362906
C    -0.927126   -0.548362    0.362641
H    -0.522174   -0.530436    1.363983
H    -1.134012   -1.532305   -0.034874
O     0.760953   -0.468441   -0.484652
O     1.618229    0.345337    0.254079

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -533.1097     91.2057    227.0998    306.5308    415.9603    470.6679    817.9757
    835.6601    918.9880   1030.2604   1084.6426   1244.5559   1263.4251   1382.3208
   1470.8280   1549.3441   3140.8926   3144.8996   3216.0621   3241.8410   3717.4656



== Thermochemistry energies (hartree) ==
  ZPVE =     0.066356  (after scaling by 0.985)
W1  Ee =  -229.586871  (total electronic energy)
W1  U0 =  -229.520514  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.211256  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.694417   -0.258022    0.043055
H     2.126977   -0.605577   -0.881634
H    -2.125997   -0.710448    0.532811
H     1.991309   -0.727872    0.967095
C     0.582893    0.704239    0.030160
H     0.404487    1.231206    0.968323
H     0.540807    1.384108   -0.822162
O    -0.200115   -0.444105   -0.124266
O    -1.875066    0.038015   -0.026199

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -753.5035     90.8140    134.8719    258.8011    400.1051    505.8126    781.5253
    838.0150    937.2796    997.2226   1166.4545   1170.4344   1203.4706   1317.1301
   1471.1226   1535.9148   3031.5855   3084.1669   3167.4547   3281.3366   3777.9256



== Thermochemistry energies (hartree) ==
  ZPVE =     0.065416  (after scaling by 0.985)
W1  Ee =  -229.589061  (total electronic energy)
W1  U0 =  -229.523646  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -229.213812  (total electronic energy)
```

Hydrocarbon 2: isopropyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.294138   -0.197180    0.002337
C    -0.000000    0.532887   -0.041105
C    -1.294138   -0.197180    0.002337
H     2.139669    0.453710   -0.221196
H     1.309964   -1.030634   -0.708112
H     1.483889   -0.641834    0.991608
H     0.000000    1.606355    0.093979
H    -1.309964   -1.030634   -0.708112
H    -2.139669    0.453710   -0.221196
H    -1.483889   -0.641835    0.991608

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    108.0142    110.0636    351.0519    390.5172    884.7674    941.2064    948.1429
   1029.2895   1146.0139   1181.1098   1371.8999   1409.4355   1414.2704   1468.3527
   1477.4209   1478.6875   1491.0577   2933.1961   2937.2405   3007.7790   3009.0800
   3082.4644   3083.5626   3167.9761


== Thermochemistry energies (hartree) ==
  ZPVE =     0.086220  (after scaling by 0.985)
W1  Ee =  -118.495776  (total electronic energy)
W1  U0 =  -118.409556  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -118.286801  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.557589   -0.849100    0.019749
C     0.367826    0.018772   -0.337445
C     0.486014    1.463512    0.108219
H     1.401385   -1.878604   -0.300108
H     1.732552   -0.841900    1.096080
H     2.451715   -0.467755   -0.473428
H     0.689245    1.522585    1.178287
H    -0.435814    2.000834   -0.107015
H     1.302902    1.950956   -0.425191
O    -0.787241   -0.604232    0.337199
O    -1.931838   -0.151722   -0.125850
H     0.142070   -0.037586   -1.402548

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     99.0371    199.7081    237.6007    302.5951    343.0845    449.4491    521.4669
    791.9765    886.3322    939.9622    950.6077   1123.5137   1153.2153   1195.9904
   1204.7216   1344.1207   1368.1951   1403.3738   1421.4108   1482.8878   1488.9614
   1494.3705   1511.5021   3036.2506   3040.9106   3062.2310   3099.6125   3109.6361
   3112.3951   3120.3661


== Thermochemistry energies (hartree) ==
  ZPVE =     0.097604  (after scaling by 0.985)
W1  Ee =  -268.972923  (total electronic energy)
W1  U0 =  -268.875319  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.527989  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.690585   -0.689674    0.023809
C     0.415876    0.074284   -0.336531
C     0.439022    1.491088    0.110637
H     1.608619   -1.728445   -0.295243
H     1.860184   -0.664931    1.100346
H     2.547635   -0.234432   -0.470990
H     0.529234    1.713122    1.166125
H     0.388342    2.311646   -0.589110
O    -0.628624   -0.676243    0.322328
O    -1.905372   -0.206703   -0.174531
H     0.238717    0.015634   -1.412699
H    -2.173658    0.396793    0.531707

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     83.4052    136.1081    217.1285    232.7340    279.5208    336.2052    456.4842
    482.5275    583.7069    829.8867    906.5006    926.8397    947.8389   1035.7493
   1154.3802   1175.6436   1319.9764   1366.9110   1378.9031   1398.3131   1458.5600
   1484.4061   1496.7041   3037.0159   3038.9094   3108.8988   3112.6193   3135.6699
   3246.0430   3747.7208


== Thermochemistry energies (hartree) ==
  ZPVE =     0.094507  (after scaling by 0.985)
W1  Ee =  -268.942482  (total electronic energy)
W1  U0 =  -268.847975  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.497205  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.506883    0.098067   -0.148522
C    -0.152156   -0.036390    0.486086
C     1.039267    0.615939   -0.060866
H    -2.078321   -0.824652   -0.035345
H    -1.413569    0.313775   -1.212601
H    -2.073128    0.903919    0.322991
O     0.827897   -0.788134   -0.239781
H    -0.154185   -0.249774    1.552381
H     1.863894    0.881375    0.592649
H     0.950765    1.214734   -0.962017

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    206.0392    366.6399    410.5318    771.8821    844.8421    907.5872    974.0105
   1042.0992   1130.0974   1156.6732   1165.3168   1188.0691   1294.1605   1407.0987
   1439.9307   1483.5220   1497.8665   1531.5306   3028.4132   3078.6941   3085.5630
   3087.1776   3109.8463   3161.6612


== Thermochemistry energies (hartree) ==
  ZPVE =     0.083856  (after scaling by 0.985)
W1  Ee =  -193.185543  (total electronic energy)
W1  U0 =  -193.101687  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -192.858655  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.230760   -0.161964    0.000017
C    -0.134285    0.452265   -0.000173
C    -1.277679   -0.219887   -0.000007
H     1.802769    0.153368    0.876702
H     1.803971    0.153838   -0.875707
H     1.179896   -1.250881   -0.000295
H    -0.166820    1.538156    0.000026
H    -1.299008   -1.303499   -0.000161
H    -2.233587    0.286535    0.000411

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    205.3893    426.3125    592.5848    924.6092    947.7973    950.8368   1030.2464
   1074.7583   1193.2901   1332.4547   1411.1422   1453.1586   1480.3100   1495.1727
   1713.2537   3014.3956   3055.4048   3091.0867   3122.4458   3129.0737   3209.1532



== Thermochemistry energies (hartree) ==
  ZPVE =     0.078210  (after scaling by 0.985)
W1  Ee =  -117.931883  (total electronic energy)
W1  U0 =  -117.853673  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -117.723135  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.107902    1.380235   -0.117394
H     0.044709    2.231466    0.551560
H    -0.078164    1.613755   -1.162745
H     1.361734    0.815538   -0.082115
C    -0.417122    0.033843    0.373739
H    -0.339473   -0.000158    1.465112
C    -1.811936   -0.342302   -0.084470
H    -2.540596    0.358274    0.324370
H    -1.878365   -0.321418   -1.171945
H    -2.070937   -1.342749    0.263113
O     1.770664   -0.308768    0.036747
O     0.507839   -0.914402   -0.189072

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2229.5380    193.6070    206.6409    316.4591    401.9669    482.9566    570.3859
    653.8259    840.7772    873.2173    922.5457    956.2967    972.8956   1092.7208
   1110.1643   1139.2020   1180.3636   1334.1392   1377.9033   1409.8930   1457.0231
   1484.4302   1496.3130   1718.6786   3009.6166   3037.1843   3090.8801   3103.0547
   3110.6763   3184.3479


== Thermochemistry energies (hartree) ==
  ZPVE =     0.091394  (after scaling by 0.985)
W1  Ee =  -268.909011  (total electronic energy)
W1  U0 =  -268.817617  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.464270  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.318352    1.405754   -0.045578
H    -0.077361    2.213988    0.636823
H    -0.660059    1.718665   -1.027834
H     0.910852    0.914651   -0.306183
C    -0.820927    0.225485    0.478778
H    -0.755081    0.060857    1.546583
C    -1.666571   -0.735539   -0.283845
H    -1.534288   -0.620544   -1.359456
H    -1.450086   -1.767406   -0.009176
H    -2.722395   -0.552349   -0.056129
O     1.794402   -0.002177   -0.295321
O     1.096038   -0.915580    0.255227

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1078.3680    149.4909    175.6899    207.7079    365.7842    420.3225    508.3866
    624.2410    636.7650    894.9108    956.1438    962.3985   1035.8341   1062.6771
   1200.0591   1287.2995   1308.5527   1317.7436   1406.7636   1442.8220   1476.7399
   1488.8662   1571.5485   1599.6502   3008.8532   3072.6314   3093.7832   3108.9174
   3161.6502   3180.5679


== Thermochemistry energies (hartree) ==
  ZPVE =     0.091390  (after scaling by 0.985)
W1  Ee =  -268.917052  (total electronic energy)
W1  U0 =  -268.825662  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.471990  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.717212    1.454957   -0.119912
H    -0.127007    2.256686    0.300522
H    -1.260894    1.658666   -1.032845
H     2.434326    0.474479   -0.368593
C    -0.671273    0.181161    0.408776
H    -0.244311    0.065758    1.396922
C    -1.649450   -0.877960   -0.004827
H    -1.939309   -0.761269   -1.049111
H    -1.223661   -1.870435    0.131882
H    -2.552731   -0.809223    0.605864
O     2.023440   -0.157469    0.238085
O     0.869209   -0.537982   -0.449193

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -502.0347     77.2151    144.3460    199.9043    296.8304    319.6959    417.2000
    440.8612    520.7855    810.8888    895.4051    942.9991    956.5096   1024.0479
   1082.1822   1191.7425   1268.2948   1380.4795   1401.4365   1434.1805   1479.7537
   1495.4993   1535.6085   3030.7300   3087.3208   3114.3451   3138.0173   3159.0095
   3231.4749   3721.2202


== Thermochemistry energies (hartree) ==
  ZPVE =     0.093795  (after scaling by 0.985)
W1  Ee =  -268.915747  (total electronic energy)
W1  U0 =  -268.821952  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.470670  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.328750   -1.111615   -0.010989
H     1.337250   -2.018033    0.573212
H     1.817421   -1.104394   -0.973549
C     0.509882    0.039305    0.410748
H     0.292989    0.046625    1.481818
C     0.866820    1.414864   -0.103616
H     1.101080    1.377743   -1.167827
H     0.023219    2.088105    0.041361
H     1.727759    1.813636    0.435997
O    -0.499496   -0.620103   -0.314111
O    -2.007577    0.169848    0.018478
H    -2.475845   -0.656969    0.197195

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -740.6327    105.6354    150.0838    203.3205    251.6169    350.5830    415.1727
    428.6591    538.0679    769.1875    845.9072    907.3394    927.5228    986.1707
   1091.8859   1166.2383   1198.0876   1288.0605   1396.4421   1422.0378   1466.9220
   1487.4752   1498.2347   3029.8699   3033.9197   3099.3422   3116.4493   3160.2450
   3275.2054   3782.5489


== Thermochemistry energies (hartree) ==
  ZPVE =     0.092884  (after scaling by 0.985)
W1  Ee =  -268.920648  (total electronic energy)
W1  U0 =  -268.827765  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -268.475958  (total electronic energy)
```

Hydrocarbon 3: isobutyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.268755   -0.679206    0.101502
C    -0.000003    0.059715   -0.346127
C    -0.000020    1.480077    0.101187
C     1.268776   -0.679160    0.101437
H    -2.166973   -0.166159   -0.245760
H    -1.316887   -0.738399    1.190674
H    -1.289134   -1.696251   -0.293322
H    -0.925833    2.030515    0.198930
H     0.925807    2.030322    0.199678
H    -0.000067    0.052067   -1.449569
H     1.317008   -0.738263    1.190615
H     2.166963   -0.166147   -0.245950
H     1.289122   -1.696240   -0.293291

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    122.6150    228.7966    253.5757    360.0523    373.7450    411.5581    542.9511
    810.2077    905.9566    947.5623    967.1558    982.2091   1091.6563   1180.4174
   1205.7344   1318.8453   1328.2073   1399.9761   1415.1436   1467.2682   1489.8184
   1493.3116   1503.5523   1511.3797   2893.7842   3019.5467   3023.4866   3080.7408
   3084.6451   3085.0696   3087.5311   3131.4525   3230.3489


== Thermochemistry energies (hartree) ==
  ZPVE =     0.114328  (after scaling by 0.985)
W1  Ee =  -157.815778  (total electronic energy)
W1  U0 =  -157.701450  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -157.537629  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.984858   -0.899222   -0.165417
C     0.742102   -0.013183   -0.287945
C    -0.357775   -0.558890    0.614675
C     1.056898    1.451677    0.021474
H     1.768017   -1.936283   -0.426410
H     2.382673   -0.884290    0.852243
H     2.773082   -0.545688   -0.830684
H     0.365338   -0.084380   -1.311772
H     1.451260    1.560560    1.034976
H     0.169099    2.077616   -0.062996
H     1.807262    1.837690   -0.669400
O    -1.609731    0.169672    0.452971
O    -2.213630   -0.153516   -0.673092
H    -0.116441   -0.429904    1.671111
H    -0.569894   -1.606855    0.407174

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     76.3854    109.0916    219.3306    234.7808    250.5676    332.9370    415.6778
    418.0864    564.9671    817.4196    873.4656    937.6780    946.8789    956.3792
    975.5436   1139.3979   1152.2855   1197.0320   1201.2073   1290.4553   1327.6167
   1376.5753   1384.3715   1407.0402   1427.6585   1476.2450   1491.5985   1496.6487
   1507.2019   1512.7898   3020.2410   3021.6721   3030.2480   3050.1113   3078.3494
   3084.5650   3093.0823   3103.3409   3108.1994


== Thermochemistry energies (hartree) ==
  ZPVE =     0.125904  (after scaling by 0.985)
W1  Ee =  -308.291652  (total electronic energy)
W1  U0 =  -308.165749  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.777334  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.747753   -1.148068   -0.170438
C     0.828672   -0.004333    0.084194
C    -0.384257   -0.177993    0.931730
C     1.258994    1.375988   -0.282916
H     1.242046   -2.107979   -0.061594
H     2.603225   -1.152270    0.522119
H     2.178246   -1.100358   -1.175375
H     2.047683    1.744907    0.390221
H     0.431620    2.083978   -0.230015
H     1.680466    1.414577   -1.291300
O    -1.580275    0.388399    0.371828
O    -1.970741   -0.435894   -0.756588
H    -0.307879    0.380120    1.875954
H    -0.563479   -1.228642    1.169149
H    -1.610767    0.072063   -1.496499

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     33.4358     70.5341    104.9496    129.9819    204.1928    235.8002    310.0464
    367.7000    400.7589    551.2879    774.8480    858.6426    939.9628    942.3565
    972.3378   1000.4202   1005.5271   1051.9266   1239.0216   1293.7248   1307.7913
   1360.1532   1376.1121   1400.4718   1416.3914   1460.1408   1469.8108   1475.6848
   1485.6146   1496.4919   2940.1077   2944.7109   2963.5689   3017.8420   3027.1571
   3053.2430   3084.9746   3089.4938   3746.8587


== Thermochemistry energies (hartree) ==
  ZPVE =     0.122531  (after scaling by 0.985)
W1  Ee =  -308.270527  (total electronic energy)
W1  U0 =  -308.147996  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.755469  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.930698   -1.279992   -0.049036
C    -0.131144    0.000000   -0.054913
C     1.237579   -0.000000   -0.582716
C    -0.930698    1.279992   -0.049036
H    -0.272060   -2.146381   -0.014050
H    -1.555426   -1.351676   -0.941587
H    -1.587027   -1.314167    0.822839
H    -1.555426    1.351676   -0.941587
H    -0.272060    2.146381   -0.014050
H    -1.587027    1.314167    0.822839
O     1.004512   -0.000000    0.830447
H     1.661345    0.916464   -0.981890
H     1.661345   -0.916464   -0.981890

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    182.2996    218.0260    356.0528    360.6338    410.6438    412.8239    700.0132
    807.9259    908.0013    923.8222    959.9394   1020.4768   1074.6552   1131.2834
   1150.3799   1172.9890   1284.2192   1391.2651   1413.0982   1423.4775   1476.3986
   1488.0208   1495.2216   1507.0339   1534.6608   3024.8752   3030.1894   3074.6200
   3079.8161   3084.9296   3109.1838   3111.0373   3155.6317


== Thermochemistry energies (hartree) ==
  ZPVE =     0.111018  (after scaling by 0.985)
W1  Ee =  -232.515736  (total electronic energy)
W1  U0 =  -232.404717  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -232.119425  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.272636   -0.676750    0.000001
C    -0.000007    0.124048    0.000004
C    -0.000110    1.454215   -0.000002
C     1.272735   -0.676582    0.000001
H    -2.153991   -0.037135    0.000036
H    -1.322215   -1.329609    0.876239
H    -1.322239   -1.329555   -0.876275
H     1.322437   -1.329441    0.876233
H     2.154004   -0.036844    0.000024
H     1.322420   -1.329365   -0.876288
H    -0.922249    2.021111   -0.000001
H     0.921944    2.021249    0.000008

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    172.8162    210.8870    381.2455    440.1560    442.7760    707.2396    814.6234
    925.1425    961.6709    988.4662   1023.0717   1086.4536   1108.9179   1297.4171
   1410.9842   1416.3024   1445.7769   1472.4631   1485.0281   1489.9416   1503.6531
   1717.8689   3007.7226   3013.3153   3048.1450   3050.8984   3101.8017   3103.4482
   3130.2230   3207.6813


== Thermochemistry energies (hartree) ==
  ZPVE =     0.105840  (after scaling by 0.985)
W1  Ee =  -157.260142  (total electronic energy)
W1  U0 =  -157.154302  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -156.981896  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.729982   -1.026856   -0.142334
C     0.632718   -0.006702   -0.035631
C    -0.496792   -0.299777    0.966070
C     1.050402    1.437910   -0.120253
H     1.333278   -2.039470   -0.223676
H     2.376129   -0.998500    0.744486
H     2.369501   -0.832714   -1.004641
H    -0.304917   -0.199741   -0.981413
H     1.667877    1.706944    0.746098
H     0.184029    2.098691   -0.128733
H     1.646542    1.629578   -1.013186
O    -1.673057    0.198285    0.336461
O    -1.550679   -0.303552   -0.986789
H    -0.402736    0.226914    1.918965
H    -0.577677   -1.377008    1.137599

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2074.1999    131.0424    187.6082    220.8176    259.6493    282.2091    363.7549
    401.9509    549.7213    660.9296    815.6935    899.6138    933.3573    948.1618
    968.9846    978.9501   1014.4557   1127.7462   1138.4629   1227.3442   1252.0236
   1282.2910   1351.4149   1400.4985   1414.2542   1471.4576   1477.7350   1491.3574
   1491.6597   1499.8779   1720.4371   2982.0842   2987.2194   3010.8712   3056.8370
   3065.2979   3066.2637   3095.5233   3106.0826


== Thermochemistry energies (hartree) ==
  ZPVE =     0.119680  (after scaling by 0.985)
W1  Ee =  -308.237025  (total electronic energy)
W1  U0 =  -308.117344  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.722677  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.103419    0.000576    1.260337
H    -0.371480   -0.915374    1.766499
H    -0.371297    0.917222    1.765367
C     0.704754    0.000003    0.129033
H    -0.335511    0.000470   -0.666622
C     1.428132   -1.286073   -0.258379
H     1.616142   -1.325179   -1.332347
H     2.396191   -1.352011    0.244308
H     0.847036   -2.167747    0.012042
C     1.429550    1.285173   -0.258734
H     1.617564    1.323813   -1.332720
H     0.849467    2.167571    0.011506
H     2.397693    1.350129    0.243910
O    -2.052038   -0.000121    0.225095
O    -1.622950    0.000500   -0.968280

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -920.2987    122.2922    179.9021    192.5073    208.2988    257.9623    366.5070
    372.9122    416.7113    546.4520    683.1347    756.3789    843.0233    943.4251
    972.8798    989.9748   1017.4941   1074.9199   1132.9713   1209.6971   1288.8704
   1327.1116   1408.8980   1414.5012   1424.5769   1483.1828   1495.0807   1498.6456
   1508.6753   1568.5048   1588.1585   3019.0304   3022.3352   3073.2892   3074.7033
   3096.5168   3097.7930   3153.4326   3239.1244


== Thermochemistry energies (hartree) ==
  ZPVE =     0.119088  (after scaling by 0.985)
W1  Ee =  -308.234418  (total electronic energy)
W1  U0 =  -308.115330  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.720203  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.070187   -0.537266    0.995685
H     0.611884    0.083767    1.694306
H     0.054349   -1.594035    1.225013
C    -0.951568    0.006922    0.245689
H     1.951756    0.770387   -1.193525
C    -1.089518    1.487428    0.083045
H    -0.922252    1.785568   -0.959046
H    -2.103726    1.817719    0.329673
H    -0.386937    2.035112    0.708192
C    -1.869988   -0.854459   -0.562024
H    -1.723492   -0.687467   -1.634888
H    -1.715286   -1.913818   -0.364020
H    -2.917461   -0.613472   -0.355460
O     1.550311   -0.751100   -0.185898
O     2.224249    0.463661   -0.317178

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -499.1799     27.6767     97.4718    120.9997    126.7134    173.2424    293.4801
    375.2122    418.0195    440.4780    456.4588    800.3667    875.0434    936.6090
    964.4024    982.8232   1031.2558   1057.0041   1070.4450   1078.0214   1310.7476
   1377.1609   1397.1779   1407.4586   1415.2549   1466.4683   1477.5072   1483.2692
   1498.4608   1555.7415   2987.5213   2998.0116   3025.3999   3032.5624   3104.3266
   3109.1281   3139.4021   3223.2736   3714.8010


== Thermochemistry energies (hartree) ==
  ZPVE =     0.121287  (after scaling by 0.985)
W1  Ee =  -308.245487  (total electronic energy)
W1  U0 =  -308.124200  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.730694  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.365522   -0.041112    0.874498
H     0.608783    0.842364    1.470600
H     0.566038   -0.954671    1.440864
C    -0.933526    0.002640    0.175068
H     2.843522    0.598261   -0.854025
C    -1.559262    1.308674   -0.158355
H    -1.916489    1.334855   -1.190242
H    -2.436990    1.476166    0.480001
H    -0.870538    2.136541   -0.003271
C    -1.611276   -1.259903   -0.218232
H    -1.992082   -1.214122   -1.240760
H    -0.946062   -2.116033   -0.128815
H    -2.478840   -1.436138    0.431844
O     0.948000   -0.035001   -0.394531
O     2.683739   -0.056126   -0.160977

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -651.7600     78.8946     96.5472    111.5576    124.7809    191.1735    203.4085
    282.9919    388.0618    402.8686    434.3460    766.4297    923.0601    935.8733
    980.8702    992.8149   1017.6637   1054.6418   1098.7156   1176.3438   1287.3300
   1315.7163   1365.3611   1403.7770   1411.1883   1459.2924   1475.4304   1477.9044
   1499.0488   1535.7380   2976.7452   2981.8922   3004.2764   3047.0586   3050.8414
   3051.2920   3116.2985   3118.9940   3785.1107


== Thermochemistry energies (hartree) ==
  ZPVE =     0.120333  (after scaling by 0.985)
W1  Ee =  -308.251537  (total electronic energy)
W1  U0 =  -308.131204  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.737022  (total electronic energy)
```

Hydrocarbon 4: tertbutyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.587488   -1.361150    0.014532
C    -0.000027   -0.000011   -0.148270
C    -1.472550    0.171814    0.014623
C     0.885071    1.189347    0.014314
H     1.581371   -1.430125   -0.433166
H    -0.043758   -2.131690   -0.433583
H     0.705018   -1.634109    1.076509
H    -1.824088    1.104079   -0.432927
H    -1.767707    0.205859    1.076623
H    -2.029355   -0.654072   -0.433583
H     1.867952    1.027801   -0.433852
H     1.062775    1.427714    1.076254
H     0.447901    2.084541   -0.433467

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    132.9968    133.2369    134.8186    262.1915    379.8252    379.9802    757.7653
    937.9257    938.0411    972.6887   1008.0016   1008.0918   1097.1729   1294.2784
   1294.3488   1397.7567   1397.8094   1425.3273   1468.5504   1471.2244   1471.3241
   1488.9202   1491.8940   1491.9784   2914.1698   2914.1873   2922.4951   3028.5368
   3028.6184   3031.6386   3070.4209   3074.9860   3075.0498


== Thermochemistry energies (hartree) ==
  ZPVE =     0.114211  (after scaling by 0.985)
W1  Ee =  -157.823966  (total electronic energy)
W1  U0 =  -157.709756  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -157.545445  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.667957    0.670834    1.265796
C     0.113820    0.350403   -0.000000
C     1.503478    0.968774    0.000000
C    -0.667957    0.670834   -1.265796
H    -0.887045    1.738171    1.304642
H    -0.093255    0.405232    2.153117
H    -1.607746    0.122322    1.280426
H     1.423454    2.055754    0.000000
H     2.062996    0.666024   -0.884767
H     2.062996    0.666024    0.884767
O     0.410249   -1.118607    0.000000
H    -0.093255    0.405232   -2.153117
H    -0.887045    1.738171   -1.304642
H    -1.607746    0.122322   -1.280426
O    -0.667957   -1.866931    0.000000

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    123.2015    180.1497    232.4116    243.0958    269.2671    331.3690    360.0768
    402.8449    437.4422    541.8098    728.8411    799.9479    929.0682    931.3197
    971.7406   1041.0430   1053.5585   1169.7132   1219.4434   1262.0575   1292.8167
   1399.5582   1402.8135   1427.7105   1471.6543   1489.4173   1490.9813   1497.9442
   1498.9160   1522.0499   3038.7158   3039.1648   3045.7611   3102.2559   3104.1263
   3110.2291   3111.6928   3120.7871   3124.6407


== Thermochemistry energies (hartree) ==
  ZPVE =     0.124586  (after scaling by 0.985)
W1  Ee =  -308.301806  (total electronic energy)
W1  U0 =  -308.177220  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.787529  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.299981   -0.417790    1.502845
C     0.398461    0.017356    0.081051
C     1.599862   -0.630154   -0.616530
C     0.416065    1.535827   -0.063131
H     0.094122    0.282969    2.298536
H     0.376328   -1.469121    1.746016
H     2.525261   -0.270029   -0.168641
H     1.599808   -0.375432   -1.676334
H     1.564555   -1.714624   -0.518454
O    -0.711641   -0.545907   -0.691519
H     0.478580    1.814196   -1.114656
H     1.276854    1.953596    0.460649
H    -0.489456    1.969532    0.356241
O    -1.968222   -0.013991   -0.203604
H    -2.273367   -0.743339    0.352216

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    109.2194    141.3243    206.9200    240.7980    252.7215    258.1678    328.1161
    353.2250    402.1434    452.2221    498.9845    601.4172    762.0479    825.1127
    913.5871    932.7689    956.2792    982.0867   1036.1685   1152.8553   1261.4030
   1274.9492   1364.9961   1394.6598   1411.1307   1460.2112   1477.8673   1488.4401
   1494.0838   1512.1049   3037.6502   3042.2023   3102.6808   3109.4591   3113.6103
   3122.9679   3136.1293   3243.2977   3753.6479


== Thermochemistry energies (hartree) ==
  ZPVE =     0.121642  (after scaling by 0.985)
W1  Ee =  -308.270613  (total electronic energy)
W1  U0 =  -308.148971  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.756034  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.930698   -1.279992   -0.049036
C    -0.131144    0.000000   -0.054913
C     1.237579   -0.000000   -0.582716
C    -0.930698    1.279992   -0.049036
H    -0.272060   -2.146381   -0.014050
H    -1.555426   -1.351676   -0.941587
H    -1.587027   -1.314167    0.822839
H    -1.555426    1.351676   -0.941587
H    -0.272060    2.146381   -0.014050
H    -1.587027    1.314167    0.822839
O     1.004512   -0.000000    0.830447
H     1.661345    0.916464   -0.981890
H     1.661345   -0.916464   -0.981890

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    182.2996    218.0260    356.0528    360.6338    410.6438    412.8239    700.0132
    807.9259    908.0013    923.8222    959.9394   1020.4768   1074.6552   1131.2834
   1150.3799   1172.9890   1284.2192   1391.2651   1413.0982   1423.4775   1476.3986
   1488.0208   1495.2216   1507.0339   1534.6608   3024.8752   3030.1894   3074.6200
   3079.8161   3084.9296   3109.1838   3111.0373   3155.6317


== Thermochemistry energies (hartree) ==
  ZPVE =     0.111018  (after scaling by 0.985)
W1  Ee =  -232.515736  (total electronic energy)
W1  U0 =  -232.404717  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -232.119425  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.272636   -0.676750    0.000001
C    -0.000007    0.124048    0.000004
C    -0.000110    1.454215   -0.000002
C     1.272735   -0.676582    0.000001
H    -2.153991   -0.037135    0.000036
H    -1.322215   -1.329609    0.876239
H    -1.322239   -1.329555   -0.876275
H     1.322437   -1.329441    0.876233
H     2.154004   -0.036844    0.000024
H     1.322420   -1.329365   -0.876288
H    -0.922249    2.021111   -0.000001
H     0.921944    2.021249    0.000008

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    172.8162    210.8870    381.2455    440.1560    442.7760    707.2396    814.6234
    925.1425    961.6709    988.4662   1023.0717   1086.4536   1108.9179   1297.4171
   1410.9842   1416.3024   1445.7769   1472.4631   1485.0281   1489.9416   1503.6531
   1717.8689   3007.7226   3013.3153   3048.1450   3050.8984   3101.8017   3103.4482
   3130.2230   3207.6813


== Thermochemistry energies (hartree) ==
  ZPVE =     0.105840  (after scaling by 0.985)
W1  Ee =  -157.260142  (total electronic energy)
W1  U0 =  -157.154302  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -156.981896  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.374528    0.007943    0.041163
C    -0.239334   -0.489943    1.355864
H    -1.472485   -0.247647    0.809877
H    -0.216368   -1.563877    1.518701
H    -0.084712    0.101532    2.251682
C     0.584397    1.520086    0.059182
H     1.318278    1.799473    0.816397
H     0.945472    1.857845   -0.911837
H    -0.352010    2.030992    0.276632
C     1.629428   -0.748555   -0.369766
H     1.437974   -1.819892   -0.408153
H     1.966037   -0.419234   -1.353630
H     2.432224   -0.560296    0.343716
O    -0.642771   -0.355494   -0.933256
O    -1.865795   -0.009016   -0.299499

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2232.9375    188.9270    195.0793    238.4295    299.3179    339.7262    392.5465
    406.8249    507.8713    569.9865    639.6141    782.1498    833.1641    905.6383
    924.3858    946.5922    972.7926   1017.4376   1042.7846   1108.3458   1173.1397
   1248.6215   1270.3820   1399.7768   1414.8222   1455.1113   1479.1162   1488.0157
   1496.2509   1509.6754   1710.7843   3034.9281   3040.1094   3094.7877   3098.0676
   3104.1973   3113.5280   3118.9170   3184.8277


== Thermochemistry energies (hartree) ==
  ZPVE =     0.118364  (after scaling by 0.985)
W1  Ee =  -308.237692  (total electronic energy)
W1  U0 =  -308.119329  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.723601  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.721059   -0.000018    0.227831
C     0.072724   -0.000113    1.458531
H    -1.179341   -0.000070    0.970425
H     0.082107   -0.915377    2.042335
H     0.082110    0.915059    2.042482
C     1.209909    1.274063   -0.387021
H     2.276798    1.395786   -0.167934
H     1.100321    1.262699   -1.471143
H     0.686663    2.141889    0.010713
C     1.209909   -1.274006   -0.387214
H     0.686638   -2.141888    0.010365
H     1.100352   -1.262464   -1.471336
H     2.276790   -1.395780   -0.168114
O    -1.246798    0.000084   -0.950567
O    -2.052458   -0.000011    0.041747

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1066.4599    129.5392    165.2107    194.0853    201.8582    204.6439    366.7876
    432.4375    433.2686    534.7269    633.6676    652.0179    816.9233    939.5041
    989.8160   1022.0894   1024.2148   1072.2748   1100.5524   1286.0098   1305.2299
   1326.8529   1409.7241   1410.8391   1425.9692   1468.9390   1480.3136   1484.5351
   1499.1572   1569.9244   1598.6130   3003.2904   3008.1821   3073.4676   3076.5548
   3091.6281   3114.7785   3117.1111   3168.6948


== Thermochemistry energies (hartree) ==
  ZPVE =     0.118558  (after scaling by 0.985)
W1  Ee =  -308.247514  (total electronic energy)
W1  U0 =  -308.128956  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.733017  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.659424    0.111180    0.154318
C     0.629958   -0.166234    1.513604
H    -2.220744    0.547831   -0.683078
H     1.001960   -1.106607    1.894172
H     0.111527    0.483571    2.204284
C     0.372785    1.513754   -0.313028
H     1.269106    2.130950   -0.215509
H     0.080859    1.524197   -1.363802
H    -0.413588    1.976165    0.282474
C     1.553931   -0.709594   -0.737671
H     1.620258   -1.738368   -0.387526
H     1.179707   -0.715055   -1.760570
H     2.561384   -0.286405   -0.747566
O    -0.945723   -0.789945   -0.372351
O    -2.115159   -0.123919    0.006574

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -487.7669     88.9942    151.7565    187.8326    203.4678    238.7849    313.5023
    383.0518    393.9403    436.9883    445.0092    514.1904    794.1423    798.9923
    937.3273    945.8456    975.7839   1020.0629   1059.3166   1077.9920   1303.4883
   1375.2400   1388.7153   1405.2746   1419.3570   1477.5224   1487.4114   1488.9793
   1508.0398   1528.5590   3025.6914   3030.9291   3078.6432   3090.0985   3106.6231
   3117.0108   3145.0795   3238.2692   3701.7344


== Thermochemistry energies (hartree) ==
  ZPVE =     0.120915  (after scaling by 0.985)
W1  Ee =  -308.243556  (total electronic energy)
W1  U0 =  -308.122642  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.729235  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.487789    0.043724    0.026149
C     1.265037   -1.196235   -0.199899
H    -2.492390   -0.559124    0.456318
H     1.565088   -1.476775   -1.197744
H     1.427753   -1.889516    0.610898
C     0.479072    0.552137    1.459441
H     1.414881    1.060642    1.694989
H    -0.343744    1.252754    1.590493
H     0.343867   -0.273327    2.158369
C     0.681171    1.144900   -1.003846
H     0.674859    0.729836   -2.011003
H    -0.133241    1.863715   -0.925230
H     1.625262    1.666943   -0.841161
O    -0.612196   -0.797319   -0.274198
O    -2.082897    0.092031   -0.129177

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -723.3235    106.4119    180.1855    192.2029    210.6768    242.7670    335.0221
    348.3646    401.7137    411.4388    480.1318    530.8473    754.2206    764.4269
    868.1073    909.8624    957.4954    983.0920   1029.0132   1036.6748   1158.7278
   1265.3814   1326.8174   1400.6343   1411.9795   1465.1336   1474.2970   1490.3417
   1498.6409   1510.3099   3034.8933   3040.6053   3100.0703   3105.1350   3116.1359
   3120.0357   3158.1296   3273.0329   3784.3896


== Thermochemistry energies (hartree) ==
  ZPVE =     0.120003  (after scaling by 0.985)
W1  Ee =  -308.251146  (total electronic energy)
W1  U0 =  -308.131144  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -307.737109  (total electronic energy)
```

Hydrocarbon 5: neopentyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.000005    1.320684   -0.753285
C     0.000000   -0.001686    0.054897
C     1.258699   -0.808909   -0.308833
C    -1.258695   -0.808916   -0.308832
C    -0.000000    0.314303    1.517295
H     0.882453    1.919408   -0.523874
H    -0.882466    1.919403   -0.523873
H    -0.000004    1.112215   -1.826312
H     0.926270    0.515943    2.038541
H    -0.926271    0.515943    2.038541
H    -2.164819   -0.254131   -0.058074
H    -1.284921   -1.756526    0.231099
H    -1.284964   -1.027242   -1.378262
H     2.164820   -0.254117   -0.058076
H     1.284969   -1.027234   -1.378263
H     1.284933   -1.756518    0.231098

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    106.5750    223.5441    271.5708    276.4896    309.0223    330.4343    389.5571
    415.5578    417.3262    554.9511    736.9411    906.1956    911.9028    947.2156
    952.2161    962.0325   1031.4285   1076.6879   1200.1347   1264.3617   1278.0764
   1391.7524   1399.1188   1419.7938   1465.5041   1480.7889   1487.2601   1489.1176
   1503.1149   1504.4361   1519.1660   3012.6404   3017.4487   3023.6726   3074.5707
   3078.5879   3083.3933   3084.2489   3088.7211   3091.1544   3127.4082   3227.6421



== Thermochemistry energies (hartree) ==
  ZPVE =     0.141668  (after scaling by 0.985)
W1  Ee =  -197.141099  (total electronic energy)
W1  U0 =  -196.999431  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -196.793722  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.063554   -1.018643   -1.089256
C    -0.747680    0.031173   -0.013335
C    -1.927658    0.145185    0.965624
C    -0.481716    1.394391   -0.666931
C     0.465868   -0.414646    0.814125
H    -1.274865   -1.992396   -0.642476
H    -0.230913   -1.139395   -1.781870
H    -1.940053   -0.718943   -1.665593
H     0.732530    0.316984    1.574524
H     0.282019   -1.386665    1.274502
H     0.361704    1.351582   -1.355179
H    -0.262106    2.157344    0.081515
H    -1.359093    1.716973   -1.229980
H    -2.140251   -0.810148    1.449619
H    -2.828532    0.455943    0.434842
H    -1.729905    0.883449    1.745090
O     1.650641   -0.622680   -0.005948
O     2.464097    0.415244    0.012654

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     67.2322     96.3604    214.3459    229.7828    260.9030    265.8219    307.0666
    335.9743    389.6075    406.1536    480.1114    553.0345    739.8855    883.4435
    912.3390    932.5342    944.4727    963.9107    968.8674   1048.3496   1085.0899
   1159.5049   1232.5810   1248.1471   1275.8564   1320.9303   1368.2178   1404.2359
   1408.3626   1437.2366   1470.6616   1483.4225   1489.3524   1491.5669   1508.8469
   1509.1239   1521.1851   3020.5321   3024.9991   3031.3061   3048.8968   3080.5358
   3084.0447   3086.2493   3091.1858   3100.3205   3104.8386   3114.9399


== Thermochemistry energies (hartree) ==
  ZPVE =      0.153045  (after scaling by 0.985)
W1  Ee =  -347.616877  (total electronic energy)
W1  U0 =  -347.463832  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -347.033300  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.090901    0.819175    1.235392
C    -0.757997   -0.072705    0.030108
C    -1.979130   -0.139922   -0.922839
C    -0.409571   -1.456614    0.477090
C     0.398603    0.558631   -0.783508
H    -1.402166    1.813394    0.910178
H    -0.224900    0.936204    1.886051
H    -1.904533    0.387887    1.820486
H     0.624035   -0.036070   -1.671569
H     0.107767    1.564181   -1.099818
H     1.928120   -0.930355    0.721946
H    -0.066123   -2.188790   -0.242015
H    -0.701939   -1.812020    1.455955
H    -2.242816    0.858228   -1.280755
H    -2.845019   -0.553635   -0.406297
H    -1.771207   -0.769336   -1.789165
O     1.593985    0.772145   -0.046966
O     2.347610   -0.462281   -0.018341

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     82.2195    145.9221    168.2912    223.1865    238.9078    258.9470    282.1709
    306.1951    341.5138    396.1744    401.9358    453.8458    553.4559    621.5174
    757.7773    867.5341    893.2415    930.4618    947.8231    956.2221   1010.9234
   1024.9251   1056.1846   1164.6371   1242.9597   1253.6327   1328.9846   1371.1282
   1389.0006   1397.1891   1417.2041   1454.5062   1469.8460   1487.3982   1492.2050
   1503.8472   1512.0371   3016.6355   3021.3596   3029.7800   3068.5296   3081.6000
   3087.7546   3098.3088   3103.4782   3126.9234   3227.6601   3662.9664


== Thermochemistry energies (hartree) ==
  ZPVE =      0.150188  (after scaling by 0.985)
W1  Ee =  -347.587649  (total electronic energy)
W1  U0 =  -347.437461  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -347.003692  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.256610    1.229964   -0.000000
C    -0.022024    0.399781   -0.000000
C    -1.263979    1.280916    0.000000
C    -0.022024   -0.751949    1.035745
C    -0.022024   -0.751949   -1.035745
H     1.305245    1.872628   -0.881946
H     2.141497    0.591900   -0.000000
H     1.305245    1.872628    0.881946
H    -0.947951   -0.860014   -1.608560
H     0.829678   -0.783053   -1.720164
H    -1.285746    1.926232   -0.881157
H    -1.285746    1.926232    0.881157
H    -2.176172    0.682589    0.000000
O     0.084107   -1.753331    0.000000
H    -0.947951   -0.860014    1.608560
H     0.829678   -0.783053    1.720164

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     34.6704    223.8302    259.8063    312.7795    343.2038    391.5052    409.3193
    637.9879    847.4178    881.6497    925.2201    940.6626    961.3668    972.6534
   1019.3739   1024.1427   1062.2610   1158.5618   1159.8996   1220.3854   1263.4308
   1293.0637   1310.6244   1375.9176   1407.4388   1427.1057   1488.2422   1491.5137
   1503.9612   1505.9809   1518.7575   1537.3345   2997.5010   3005.9835   3014.7488
   3021.8248   3043.5209   3044.2681   3071.5826   3076.7520   3085.2035   3087.0035



== Thermochemistry energies (hartree) ==
  ZPVE =     0.139932  (after scaling by 0.985)
W1  Ee =  -271.834575  (total electronic energy)
W1  U0 =  -271.694643  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -271.369407  (total electronic energy)
```

Species 5: dimethylcyclopropane

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.969464    1.272901    0.000006
C    -0.149643    0.000000    0.000167
C    -0.969464   -1.272901    0.000006
C     1.153212    0.000000    0.755277
C     1.153112    0.000000   -0.755332
H    -1.612454    1.325254   -0.882306
H    -0.331866    2.157967   -0.000111
H    -1.612462    1.325504    0.882303
H    -1.612454   -1.325254   -0.882306
H    -1.612462   -1.325504    0.882303
H    -0.331866   -2.157967   -0.000111
H     1.451600    0.908105   -1.261682
H     1.451600   -0.908105   -1.261682
H     1.451924   -0.908136    1.261424
H     1.451924    0.908136    1.261424

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    218.1382    242.1242    328.7420    352.8845    362.1249    396.1359    685.2570
    791.7205    847.8843    902.0329    943.3228    946.5531    976.2402   1042.3030
   1066.9208   1077.7220   1086.0058   1159.4654   1188.8213   1317.6411   1350.8070
   1413.6465   1426.2415   1472.6796   1483.9442   1495.7395   1502.0405   1504.9862
   1518.9348   3009.5786   3014.4939   3060.7114   3063.6203   3082.4996   3084.6356
   3116.4707   3120.9059   3189.3727   3203.5157


== Thermochemistry energies (hartree) ==
  ZPVE =     0.134745  (after scaling by 0.985)
W1  Ee =  -196.572485  (total electronic energy)
W1  U0 =  -196.437740  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -196.224590  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.707075    0.050851    0.025572
C     0.154903    1.383846    0.478728
H     0.347332    1.680071    1.505029
H     0.214681    2.201897   -0.234343
H    -1.210426    1.104396    0.420922
C     1.062317   -0.825013    1.235364
H     0.185503   -1.005972    1.856105
H     1.454887   -1.791986    0.915548
H     1.822977   -0.341219    1.849769
C     1.940430    0.246386   -0.878643
H     2.313099   -0.715685   -1.237053
H     1.703309    0.863991   -1.746031
H     2.745683    0.733762   -0.328522
C    -0.386113   -0.666027   -0.823831
H    -0.571399   -0.122368   -1.753789
H    -0.088067   -1.691569   -1.047738
O    -2.134812    0.520714    0.033612
O    -1.588845   -0.777662   -0.086492

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1672.4632    105.8628    230.0798    248.5721    274.1338    306.2501    326.2725
    391.1029    433.2567    454.6837    487.6370    539.6671    644.9972    759.4820
    876.7261    911.0838    939.2342    943.4082    972.6930    998.5053   1028.7185
   1045.9490   1074.1655   1117.6902   1200.3641   1224.6274   1244.4312   1311.4523
   1358.8324   1399.8725   1419.5323   1459.3651   1472.1839   1489.4159   1495.6086
   1505.2608   1511.9057   1570.6164   3019.3201   3023.1685   3029.7630   3081.5034
   3083.8540   3085.4367   3089.7680   3095.8197   3106.0438   3170.1797


== Thermochemistry energies (hartree) ==
  ZPVE =     0.147113  (after scaling by 0.985)
W1  Ee =  -347.571564  (total electronic energy)
W1  U0 =  -347.424451  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -346.987990  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.016496   -0.000793   -0.943532
H     0.409906    0.916804   -1.348344
H     0.409603   -0.919094   -1.347051
C    -1.128907    0.000008   -0.043670
C    -0.007352    0.000148    1.028353
H    -0.049984   -0.908539    1.624928
H     1.192763    0.000642    0.787506
H    -0.050297    0.908853    1.624921
C    -1.974654   -1.266502   -0.048660
H    -2.616557   -1.302601    0.833167
H    -2.613607   -1.300842   -0.933170
H    -1.350665   -2.160919   -0.048926
O     2.618644    0.000750    0.594962
O     2.588442   -0.000728   -0.681852
C    -1.973893    1.267014   -0.049885
H    -2.612792    1.300890   -0.934468
H    -2.615820    1.304310    0.831892
H    -1.349379    2.161083   -0.050963

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1149.5548     50.2724     82.9078    154.7102    229.5117    239.6510    291.2708
    326.9980    343.8853    395.6228    428.9280    464.9554    469.0334    723.1280
    755.4133    846.1835    864.5661    925.3238    958.5918    966.8998    984.6299
   1011.0452   1044.2671   1070.0913   1187.7166   1269.7627   1300.7233   1342.5006
   1408.0932   1421.9730   1427.7414   1432.0527   1480.5246   1487.5065   1493.8580
   1506.7016   1514.7382   1707.5408   3022.1756   3026.7741   3047.8462   3083.3572
   3087.8601   3092.2915   3094.7118   3143.1901   3184.3910   3289.3227


== Thermochemistry energies (hartree) ==
  ZPVE =     0.145145  (after scaling by 0.985)
W1  Ee =  -347.502385  (total electronic energy)
W1  U0 =  -347.357240  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -346.919350  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.051209   -0.043657    0.026330
C     0.169407    0.214992    1.186033
H     0.051473    1.212997    1.575672
H    -0.451165   -0.567179    1.591307
H    -3.046455   -0.660042   -0.764728
C     1.519893   -1.490496   -0.096900
H     0.686921   -2.184282    0.020926
H     1.975006   -1.667346   -1.073471
H     2.260633   -1.718789    0.671455
C     2.195469    0.953427   -0.129967
H     2.675026    0.843888   -1.104514
H     1.838374    1.980234   -0.041325
H     2.949628    0.791362    0.642497
C    -0.163545    0.277914   -0.793791
H    -0.172105    1.238666   -1.287269
H    -0.604517   -0.543551   -1.338868
O    -2.668841   -0.481428    0.107766
O    -1.930837    0.706548   -0.113004

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -682.6153     53.2290     65.9449    218.6590    229.7941    242.4906    284.2312
    332.6664    351.0875    378.1500    392.1771    414.1708    454.2027    581.4693
    699.1829    753.2800    848.3401    897.1624    924.4887    932.6014    962.2642
   1027.5657   1032.2454   1067.8991   1093.5767   1192.8272   1296.7841   1309.3465
   1355.1427   1404.4073   1415.7479   1432.2422   1477.3386   1487.1305   1490.5616
   1504.3633   1509.1494   3020.0294   3024.8682   3081.9028   3086.3899   3090.2861
   3094.2881   3124.5072   3170.6565   3231.1471   3279.9067   3718.9681


== Thermochemistry energies (hartree) ==
  ZPVE =      0.148182  (after scaling by 0.985)
W1  Ee =  -347.506284  (total electronic energy)
W1  U0 =  -347.358101  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -346.922922  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.906396   -0.004647   -0.007550
C     0.403864   -0.272665    1.392132
H     0.316899   -1.292238    1.741558
H     0.407140    0.502206    2.144696
H    -3.275789   -0.488035    0.270088
C     1.991509   -0.988273   -0.456328
H     1.665813   -2.021779   -0.330878
H     2.235009   -0.837970   -1.510159
H     2.906540   -0.848012    0.121808
C     1.382912    1.444141   -0.147539
H     1.667054    1.658703   -1.178898
H     0.592875    2.139070    0.138728
H     2.250733    1.632043    0.487515
C    -0.437976   -0.216282   -0.725362
H    -0.661212    0.513542   -1.504364
H    -0.551787   -1.224551   -1.133629
O    -2.816356    0.094721   -0.348284
O    -1.312832   -0.033049    0.400961

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -779.6758     69.1582    121.0792    155.5432    213.4047    240.5013    280.7748
    314.8897    326.8760    397.7864    414.1187    428.6868    535.3341    565.6617
    778.9146    829.1723    907.8743    923.6847    956.1848    969.5396    995.7464
   1003.9663   1058.3862   1093.2361   1186.8764   1224.5991   1242.1801   1284.5027
   1346.5597   1402.6298   1419.1037   1470.1641   1489.0961   1491.1290   1504.3355
   1512.0771   1523.5266   3010.6206   3020.4076   3026.5377   3070.4740   3081.2668
   3087.1387   3089.5113   3097.0692   3138.4276   3241.1295   3790.5885


== Thermochemistry energies (hartree) ==
  ZPVE =     0.148845  (after scaling by 0.985)
W1  Ee =  -347.557801  (total electronic energy)
W1  U0 =  -347.408955  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -346.974577  (total electronic energy)
```

Hydrocarbon 6: cyclohexyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.285611   -0.776670    0.155807
C    -0.000018   -1.460529   -0.162801
C    -1.285630   -0.776640    0.155807
C    -1.264955    0.710844   -0.240619
C     0.000017    1.408445    0.267198
C     1.264973    0.710813   -0.240619
H     2.156968    1.210222    0.143880
H     1.303304    0.789616   -1.331113
H     0.000017    1.407584    1.362970
H     0.000030    2.456287   -0.041544
H    -2.156938    1.210274    0.143879
H    -1.303282    0.789647   -1.331113
H    -1.477514   -0.834498    1.241601
H    -2.125418   -1.287915   -0.319242
H    -0.000036   -2.516295   -0.400319
H     2.125386   -1.287967   -0.319240
H     1.477492   -0.834532    1.241601

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    171.7952    208.1574    325.0412    391.0507    438.7415    459.0014    610.1012
    781.8569    804.8087    854.4815    869.9876    874.5867    926.3200   1014.8169
   1032.8107   1056.1635   1096.2443   1112.9207   1129.7121   1151.8428   1254.1347
   1282.6884   1294.9830   1340.5850   1351.9578   1352.2727   1378.3623   1391.6388
   1397.1527   1467.6569   1472.2412   1490.3116   1493.3079   1503.7239   2892.2698
   2897.0248   2996.3819   3011.3840   3012.3755   3044.8108   3046.4316   3049.1622
   3050.4108   3054.6026   3164.3272


== Thermochemistry energies (hartree) ==
  ZPVE =     0.152593  (after scaling by 0.985)
W1  Ee =  -235.263378  (total electronic energy)
W1  U0 =  -235.110785  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -234.846696  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.119638    1.155889   -0.276634
C    -0.645763   -0.178900    0.231288
C     0.231637   -1.348214   -0.185092
C     1.675324   -1.126332    0.284971
C     2.231458    0.214877   -0.203477
C     1.320679    1.379003    0.199237
H     1.699481    2.318348   -0.207215
H     1.330731    1.487456    1.288548
H     2.325092    0.191081   -1.293929
H     3.237413    0.369413    0.191726
H     2.302704   -1.948923   -0.062342
H     1.707338   -1.154241    1.378824
H     0.205799   -1.435338   -1.275015
H    -0.170493   -2.277510    0.221203
H    -0.776089   -0.151626    1.314687
O    -1.980637   -0.436210   -0.323281
O    -2.906136    0.301090    0.254242
H    -0.777207    1.955824    0.064176
H    -0.152766    1.148533   -1.370114

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     81.1545    130.6329    224.5551    252.9058    322.6707    365.0373    441.3029
    455.4165    506.7986    565.5207    799.0743    806.9319    847.1910    897.4338
    899.4400    918.6785    938.6364   1018.4923   1046.3655   1067.4776   1090.5707
   1100.4070   1172.3633   1186.5406   1213.6701   1273.3250   1286.3746   1290.6021
   1332.1647   1340.1457   1368.7684   1377.4263   1379.2436   1384.2980   1396.4021
   1490.8745   1492.4407   1495.3904   1500.8036   1513.7810   3004.2342   3008.3862
   3014.7293   3021.9232   3024.6455   3049.9925   3057.3473   3060.0779   3063.4413
   3073.8966   3084.0187


== Thermochemistry energies (hartree) ==
  ZPVE =     0.163214  (after scaling by 0.985)
W1  Ee =  -385.741148  (total electronic energy)
W1  U0 =  -385.577934  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.088450  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.624685   -0.207931    0.245677
C     0.313967   -1.351706   -0.157268
C     1.748666   -1.064431    0.298789
C     2.266775    0.261398   -0.262880
C     1.343548    1.430535    0.124347
C    -0.087158    1.121347   -0.152553
H    -0.787815    1.899876   -0.416331
H     1.643710    2.345333   -0.389472
H     1.484706    1.634034    1.199739
H     2.319516    0.193643   -1.352921
H     3.280881    0.453762    0.093371
H     2.398212   -1.885427   -0.010724
H     1.785838   -1.036560    1.392994
H     0.283462   -1.450436   -1.245014
H    -0.051921   -2.287905    0.266534
O    -1.878998   -0.514603   -0.373770
O    -2.863109    0.438170    0.110524
H    -3.414631   -0.142565    0.651480
H    -0.771779   -0.247569    1.339654

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     96.1273    118.7914    186.0180    202.7855    241.9066    314.4685    347.1631
    372.6427    456.3801    491.4717    530.3264    607.5270    793.4726    838.3919
    868.0652    902.8012    907.4420    940.4775    965.6743   1035.0423   1057.6489
   1070.5289   1103.4948   1111.7295   1149.0862   1205.4523   1258.6561   1278.3585
   1314.6222   1328.7898   1347.2849   1351.5667   1363.8920   1375.0533   1382.3228
   1398.8538   1472.8184   1491.8575   1495.6451   1504.5781   2882.7603   2902.2527
   3003.8314   3018.5884   3030.9419   3054.0264   3056.1840   3059.6996   3074.9549
   3197.2121   3757.6729


== Thermochemistry energies (hartree) ==
  ZPVE =     0.160036  (after scaling by 0.985)
W1  Ee =  -385.714406  (total electronic energy)
W1  U0 =  -385.554370  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.061174  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.987865    0.830017   -0.295546
C     0.338182    1.513787   -0.029632
C     1.547150    0.577683   -0.171576
C     1.284886   -0.801403    0.436723
C     0.132646   -1.506742   -0.286444
C    -1.089957   -0.632089   -0.413301
H    -1.903971   -1.044883   -1.004487
O    -1.522839    0.034823    0.777730
H    -0.139107   -2.431682    0.228912
H     0.446924   -1.792508   -1.295933
H     1.039678   -0.697354    1.495598
H     2.183409   -1.417868    0.376827
H     2.423439    1.038355    0.287912
H     1.783634    0.453531   -1.233188
H     0.299624    1.930038    0.980625
H     0.442356    2.361959   -0.709699
H    -1.743528    1.434301   -0.789754

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    142.2384    270.9763    357.0682    375.4289    442.0543    543.0545    648.0426
    767.0409    783.5150    828.9652    845.8561    892.1641    901.0616    985.6822
   1005.5096   1043.5738   1051.9402   1080.3551   1101.6736   1171.7515   1194.6803
   1211.0727   1278.1059   1289.9235   1304.6263   1359.9821   1372.0992   1377.2940
   1391.6798   1400.6856   1462.9074   1481.4607   1486.2204   1494.7198   1503.1804
   3005.9421   3008.2551   3022.8069   3031.8334   3045.4776   3054.1430   3062.1978
   3071.9646   3088.5348   3103.5144


== Thermochemistry energies (hartree) ==
  ZPVE =     0.148870  (after scaling by 0.985)
W1  Ee =  -309.958304  (total electronic energy)
W1  U0 =  -309.809434  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -309.423628  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.493240    0.048413    0.109913
C     0.662624    1.302204    0.056893
C    -0.662622    1.302205   -0.056894
C    -1.493241    0.048415   -0.109910
C    -0.696924   -1.189909    0.315775
C     0.696922   -1.189909   -0.315777
H     1.240457   -2.098105   -0.048371
H     0.595292   -1.193818   -1.405178
H    -0.595293   -1.193822    1.405176
H    -1.240459   -2.098104    0.048367
H    -2.375187    0.166413    0.526004
H    -1.883533   -0.086031   -1.126065
H    -1.191963    2.247292   -0.112713
H     1.191967    2.247290    0.112709
H     1.883527   -0.086035    1.126070
H     2.375190    0.166409   -0.525997

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    165.0329    275.1674    401.6350    457.5924    502.9580    656.4664    732.0702
    821.8436    828.8011    880.9519    909.8226    936.3328   1007.0416   1020.0417
   1047.7464   1071.5715   1100.8874   1161.9743   1163.8994   1250.5929   1270.9635
   1295.0380   1360.2879   1370.9567   1371.5383   1387.0763   1426.7188   1476.8697
   1482.9182   1494.9827   1503.2465   1715.2585   2986.6406   2986.7016   3007.3717
   3013.9008   3030.0963   3030.7614   3056.0484   3058.4174   3127.2057   3150.7630



== Thermochemistry energies (hartree) ==
  ZPVE =     0.143607  (after scaling by 0.985)
W1  Ee =  -234.702725  (total electronic energy)
W1  U0 =  -234.559118  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -234.286061  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.302689    0.937921    0.315330
C     0.612007   -0.436474   -0.257855
C    -0.422156   -1.453410    0.192521
C    -1.801921   -0.940327   -0.265911
C    -2.106258    0.492955    0.201763
C    -0.988961    1.505499   -0.181212
H    -1.208358    2.480545    0.254962
H    -0.968000    1.624688   -1.268009
H    -2.223466    0.501892    1.288791
H    -3.056951    0.825968   -0.219148
H    -2.580763   -1.613882    0.095171
H    -1.846408   -0.978103   -1.358384
H    -0.389469   -1.552663    1.279932
H    -0.216256   -2.435542   -0.236890
H     0.622633   -0.375484   -1.353170
O     1.938293   -0.681050    0.200071
O     2.597731    0.517321   -0.186821
H     1.595818    1.236205   -0.019179
H     0.410628    0.959225    1.402103

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2178.1664    156.3939    211.5943    288.0581    315.8147    336.7960    396.7274
    469.5729    509.6141    582.0763    658.8706    797.6305    821.5081    837.0219
    892.3221    910.5860    930.6988    947.7515    974.1276   1040.5129   1051.9244
   1059.1881   1094.9272   1147.8896   1170.4303   1190.7421   1200.6941   1262.4362
   1268.0694   1309.4695   1336.0935   1343.4117   1365.1512   1374.7062   1388.1256
   1398.3576   1489.5444   1492.5293   1498.5046   1506.3188   1737.0515   2981.6498
   3015.2339   3019.6568   3023.0462   3031.6298   3054.9007   3061.3475   3065.0021
   3074.7051   3078.9996


== Thermochemistry energies (hartree) ==
  ZPVE =     0.157460  (after scaling by 0.985)
W1  Ee =  -385.676154  (total electronic energy)
W1  U0 =  -385.518694  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.023595  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.361491    0.385879    1.042979
C    -0.167309   -0.970851    0.789359
C     1.030451   -1.450090   -0.042901
C     2.043260   -0.335459   -0.329491
C     1.339879    0.965970   -0.720671
C     0.471918    1.466940    0.434949
H    -0.162583    2.300359    0.127689
H     1.116708    1.862750    1.231929
H     0.713659    0.796040   -1.600681
H     2.067298    1.731471   -0.994921
H     2.731150   -0.652928   -1.114941
H     2.649600   -0.154238    0.563759
H     0.681572   -1.868590   -0.991131
H     1.521592   -2.271039    0.482199
H    -0.496639   -1.648751    1.573929
O    -2.222550   -0.611363   -0.698211
O    -2.119991    0.602407   -0.324901
H    -1.011701    0.676708    1.857139
H    -1.210579   -1.074462    0.004559

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -970.0540     82.6772    122.6384    197.6235    215.8693    305.2980    382.8677
    444.1321    469.1231    542.9228    659.6322    715.6243    797.9577    821.5627
    824.9761    882.6773    906.1261    946.0279    976.7028   1027.4372   1051.0282
   1072.3713   1109.3340   1151.2179   1182.2528   1237.0721   1275.7602   1290.0458
   1306.2665   1317.6166   1357.9196   1369.3722   1375.4279   1385.8844   1408.7133
   1459.6318   1492.3522   1498.2637   1507.4051   1558.8811   1572.7744   2971.7847
   3005.0488   3015.5359   3025.2248   3053.7986   3054.7274   3062.2286   3066.8253
   3095.6018   3173.9225


== Thermochemistry energies (hartree) ==
  ZPVE =     0.156690  (after scaling by 0.985)
W1  Ee =  -385.683105  (total electronic energy)
W1  U0 =  -385.526416  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.030289  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     0.029951    0.962133   -0.853940
C     0.434622   -0.363423   -0.804010
C    -0.505905   -1.438999   -0.306554
C    -1.888924   -0.901392    0.083623
C    -1.766701    0.429757    0.825857
C    -1.137686    1.489166   -0.084731
H    -0.834498    2.367217    0.495942
H    -1.889080    1.865509   -0.792922
H    -1.137049    0.292727    1.708637
H    -2.741912    0.770273    1.177461
H    -2.411248   -1.638842    0.695093
H    -2.496133   -0.754115   -0.814839
H    -0.036493   -1.929318    0.549939
H    -0.600992   -2.206770   -1.077600
H     1.190555   -0.677534   -1.510165
O     1.656730   -0.377746    0.642949
O     2.896071    0.147336    0.249105
H     2.902757    1.018094    0.670068
H     0.639537    1.672583   -1.399520

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -482.5643     59.2492     91.8931    143.6848    198.3686    283.6295    334.5486
    358.2804    409.4347    461.5376    499.3316    675.7740    722.3976    808.6234
    821.3977    881.8042    887.9400    911.3757    948.1380   1012.7954   1052.2070
   1061.3716   1067.4757   1084.8461   1154.5620   1164.5737   1223.1642   1263.7726
   1295.8285   1358.2692   1368.2525   1369.1793   1373.1519   1386.7752   1422.3626
   1458.4330   1476.7642   1497.0847   1503.8992   1508.7299   2962.5103   3002.5977
   3009.6661   3025.8077   3029.1575   3052.5848   3064.0678   3067.3963   3148.9229
   3172.6420   3724.3992


== Thermochemistry energies (hartree) ==
  ZPVE =     0.159011  (after scaling by 0.985)
W1  Ee =  -385.687646  (total electronic energy)
W1  U0 =  -385.528635  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.034617  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.295192   -1.232519    0.717086
C     0.609076   -0.066475    0.822298
C     0.018636    1.322598    0.566035
C    -1.418918    1.300853    0.019586
C    -1.669403    0.107908   -0.904495
C    -1.512709   -1.205583   -0.130227
H    -1.527423   -2.071085   -0.799992
H    -2.380167   -1.344634    0.533992
H    -0.958887    0.124756   -1.732453
H    -2.671005    0.159466   -1.333953
H    -1.626862    2.236793   -0.501010
H    -2.127961    1.249885    0.852433
H     0.691966    1.811907   -0.138111
H     0.055237    1.903479    1.489434
H     1.248264   -0.082091    1.707832
O     1.269023   -0.635776   -0.287158
O     2.687404    0.295788   -0.609733
H     3.261513   -0.480163   -0.655510
H    -0.005032   -2.149101    1.210772

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -682.2688     70.4393    124.0898    139.2454    154.1480    264.0097    289.2933
    380.0902    408.7250    456.9549    520.2651    663.3137    704.4083    798.3671
    816.9442    850.9887    872.3261    888.8443    957.1673    997.8799   1007.9818
   1050.1419   1057.3020   1083.0810   1143.1282   1171.0744   1198.0060   1259.5371
   1290.0996   1305.4877   1359.6124   1361.3637   1365.0399   1389.0275   1407.4392
   1416.3649   1454.1175   1485.2250   1496.2610   1504.8415   2941.5466   3002.8438
   3016.4412   3025.3572   3040.3076   3046.2904   3060.5019   3077.6156   3087.5863
   3189.8777   3787.3882


== Thermochemistry energies (hartree) ==
  ZPVE =     0.158063  (after scaling by 0.985)
W1  Ee =  -385.693129  (total electronic energy)
W1  U0 =  -385.535066  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.040470  (total electronic energy)
```

Hydrocarbon 7: cyclohexenyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.270924   -0.670120    0.194373
C    -1.211941    0.815216    0.003325
C     0.001758    1.472759   -0.092155
C     1.213897    0.812327    0.003290
C     1.269313   -0.673149    0.194400
C    -0.001619   -1.357184   -0.327410
H    -0.002886   -2.414228   -0.056089
H    -0.001543   -1.307736   -1.419272
H     1.397519   -0.901934    1.261986
H     2.151420   -1.087820   -0.300069
H     2.140012    1.370470   -0.036080
H     0.003020    2.547855   -0.231153
H    -2.136708    1.375592   -0.036047
H    -2.154005   -1.082653   -0.300149
H    -1.399736   -0.898646    1.261941

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    181.9479    252.8795    433.0617    503.5292    516.4283    606.2741    695.2877
    730.3359    833.1947    862.9551    890.0484    956.0233    966.2615   1017.2937
   1056.1173   1063.7804   1138.9134   1146.1474   1164.7025   1217.9102   1271.5977
   1345.9751   1361.7991   1371.5230   1403.6826   1450.0302   1476.2952   1479.3779
   1495.3697   1514.5125   2954.3821   2955.7192   3019.9092   3033.4492   3040.1445
   3063.4971   3142.5272   3168.1560   3177.1282


== Thermochemistry energies (hartree) ==
  ZPVE =     0.130057  (after scaling by 0.985)
W1  Ee =  -234.057321  (total electronic energy)
W1  U0 =  -233.927263  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -233.640816  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.143523   -0.296366   -0.248241
C    -1.626244    1.106064   -0.109575
C    -0.374439    1.406148    0.227564
C     0.645448    0.361421    0.551672
C     0.060998   -1.034477    0.719939
C    -1.011870   -1.323667   -0.329382
H    -1.404954   -2.332968   -0.201763
H    -0.558893   -1.282580   -1.322588
H    -0.370013   -1.097105    1.723392
H     0.874897   -1.758364    0.678121
H    -0.055204    2.438893    0.289131
H    -2.329465    1.911264   -0.292153
H    -2.782586   -0.360730   -1.132434
H    -2.800309   -0.517476    0.602293
O     1.619649    0.367894   -0.576597
H     1.239765    0.640911    1.421258
O     2.740918   -0.237466   -0.253043

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     76.0001    109.3942    216.5448    265.6829    340.9194    438.1198    455.6590
    529.1480    567.5532    696.0192    738.0811    824.1990    832.2187    885.5125
    905.1720    945.6874   1015.9000   1018.9935   1064.9139   1074.9161   1109.6045
   1166.2429   1177.8565   1184.6488   1262.1925   1281.3140   1327.0037   1357.5983
   1368.5749   1376.2787   1395.8683   1432.7734   1472.9319   1487.4254   1500.4707
   1709.8220   2989.0206   3022.7491   3032.4098   3044.7428   3069.7347   3074.1628
   3083.3531   3140.8394   3169.4221


== Thermochemistry energies (hartree) ==
  ZPVE =     0.139661  (after scaling by 0.985)
W1  Ee =  -384.508858  (total electronic energy)
W1  U0 =  -384.369197  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.856462  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.269576   -0.270483   -0.096576
C    -1.682249    1.110892   -0.086820
C    -0.401712    1.371823    0.158875
C     0.603526    0.310707    0.499210
C     0.021357   -1.055141    0.539334
C    -1.191467   -1.354318   -0.268318
H    -1.592942   -2.338914   -0.026702
H    -0.916926   -1.386772   -1.334196
H     0.589827   -1.850166    1.001169
H    -0.030725    2.388525    0.140653
H    -2.359938    1.935364   -0.279151
H    -3.012008   -0.350157   -0.894120
H    -2.817085   -0.434646    0.838365
O     1.632009    0.442182   -0.537671
H     1.101620    0.554259    1.441966
O     2.831816   -0.216822   -0.055204
H     2.848303   -1.001250   -0.619217

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     67.1887    117.2789    176.8257    240.7993    246.6007    297.5087    374.7432
    452.4996    501.8589    553.0556    587.4548    716.5016    759.9715    837.6426
    883.7487    896.8407    922.7228    959.1561    985.6141   1008.2566   1036.1460
   1066.6177   1128.4758   1177.0111   1189.1308   1271.3026   1305.1606   1317.5783
   1356.5852   1358.9750   1378.3950   1401.3927   1428.4045   1468.7809   1481.3135
   1712.4954   2930.0516   3000.3835   3017.6831   3044.0254   3065.1211   3140.9802
   3173.6311   3182.3496   3758.7556


== Thermochemistry energies (hartree) ==
  ZPVE =     0.136832  (after scaling by 0.985)
W1  Ee =  -384.483308  (total electronic energy)
W1  U0 =  -384.346476  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.830386  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.605525   -0.558623    0.098808
C    -1.372721    0.910958   -0.128619
C    -0.179572    1.485859   -0.001383
C     1.010556    0.700217    0.402356
C     0.928872   -0.762490    0.363199
C    -0.350462   -1.419947   -0.127387
H    -0.476049   -2.390560    0.354813
H    -0.228873   -1.608485   -1.195466
H    -0.054794    2.548371   -0.170250
H    -2.233943    1.514663   -0.391422
H    -2.408910   -0.908495   -0.552258
H    -1.979348   -0.697344    1.120194
O     1.696453   -0.054217   -0.621508
H     1.684656    1.174652    1.109306
H     1.538754   -1.334900    1.055303

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    110.8949    251.9600    396.5646    485.1589    504.2510    542.6020    712.7121
    760.7092    789.7555    821.3025    867.1795    938.3363    963.6737    976.4022
   1005.6381   1048.4479   1060.7655   1090.3557   1152.3957   1197.3324   1219.0463
   1274.4125   1286.8170   1348.1525   1359.2491   1395.9813   1427.8540   1458.9387
   1478.9254   1487.5854   1705.5101   2992.9448   3037.3061   3052.6807   3075.4345
   3104.4803   3115.0507   3142.7394   3167.5092


== Thermochemistry energies (hartree) ==
  ZPVE =     0.125231  (after scaling by 0.985)
W1  Ee =  -308.722842  (total electronic energy)
W1  U0 =  -308.597611  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -308.188411  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.190453   -0.728182   -0.241210
C     0.113603   -1.419299    0.063434
C     1.254089   -0.723538    0.106387
C     1.254089    0.723538   -0.106387
C     0.113603    1.419299   -0.063434
C    -1.190453    0.728182    0.241210
H    -2.028422    1.269349   -0.200715
H    -1.351022    0.756441    1.327964
H     0.117014    2.495348   -0.184809
H     2.198996   -1.223417    0.278247
H     0.117013   -2.495348    0.184809
H    -2.028422   -1.269349    0.200715
H    -1.351022   -0.756441   -1.327964
H     2.198996    1.223417   -0.278247

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    192.8098    302.3568    481.7906    523.8932    574.1460    674.6680    764.4143
    781.3944    853.3941    930.4329    963.3190    981.5269    996.0674   1015.2611
   1046.6052   1069.1296   1175.3067   1191.3360   1205.2056   1269.4904   1359.6232
   1363.2187   1405.9565   1443.7607   1471.7013   1482.0943   1637.3882   1703.4535
   2957.5285   2971.0729   3057.7442   3058.6910   3148.6677   3155.3902   3170.1798
   3179.4596


== Thermochemistry energies (hartree) ==
  ZPVE =     0.120185  (after scaling by 0.985)
W1  Ee =  -233.474518  (total electronic energy)
W1  U0 =  -233.354333  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -233.058055  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.030809   -0.573900   -0.158577
C    -1.766664    0.904443   -0.142938
C    -0.585019    1.449468    0.137518
C     0.606261    0.625806    0.513538
C     0.291000   -0.858085    0.710485
C    -0.727351   -1.397498   -0.251784
H    -0.930928   -2.452159   -0.068235
H    -0.342618   -1.302824   -1.269944
H     0.202073   -1.191302    1.741654
H     1.569264   -1.096464    0.287453
H    -0.459078    2.525020    0.127670
H    -2.605473    1.552933   -0.370628
H    -2.682138   -0.821716   -1.000144
H    -2.589181   -0.851890    0.742359
O     1.561521    0.636275   -0.575806
H     1.097259    1.021835    1.407694
O     2.440518   -0.421879   -0.230110

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2159.9649    114.2653    192.5710    244.2835    289.2540    429.1863    461.1906
    521.9295    586.8638    677.9427    728.0027    744.1971    825.2366    850.4932
    883.2391    920.3935    943.4556    972.3340    992.3649   1010.9271   1050.6843
   1071.3579   1106.8958   1137.6790   1172.7863   1218.7674   1257.0187   1309.8600
   1321.2501   1354.0180   1368.1685   1394.1768   1423.3472   1476.0250   1492.3647
   1701.3982   1717.0308   3001.3496   3013.1543   3030.8031   3047.2850   3082.1471
   3113.4017   3141.3124   3168.1794


== Thermochemistry energies (hartree) ==
  ZPVE =      0.133649  (after scaling by 0.985)
W1  Ee =  -384.450007  (total electronic energy)
W1  U0 =  -384.316359  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.797757  (total electronic energy)
```

Species 8: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.125361   -0.435280   -0.277739
C    -1.694591    0.998372   -0.415041
C    -0.557272    1.443838    0.139189
C     0.262574    0.549435    0.923548
C     0.154154   -0.834316    0.795816
C    -0.922849   -1.376570   -0.153408
H    -1.247129   -2.362984    0.177272
H    -0.488959   -1.512423   -1.148261
H     0.394519   -1.429736    1.673367
H     1.286952   -0.977118    0.142258
H    -0.275978    2.486035    0.070720
H    -2.351750    1.687781   -0.931091
H    -2.738158   -0.728497   -1.131968
H    -2.779015   -0.519168    0.600559
O     2.239223    0.649215   -0.371979
H     0.877480    0.972155    1.705274
O     2.338541   -0.610330   -0.532060

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -1078.2646     97.5341    126.8272    177.6611    210.5703    286.0263    399.9607
    497.8871    528.7688    586.5982    656.0732    723.0531    762.6606    845.8168
    850.8196    924.3539    963.8049    993.4353    997.1791   1007.4732   1063.5988
   1072.7155   1175.6094   1187.2790   1221.4283   1261.9647   1294.7437   1318.9657
   1357.7863   1365.5877   1399.3008   1438.3204   1472.6538   1492.5637   1534.1243
   1562.9257   1657.0727   2976.5881   3015.1670   3057.2926   3074.1742   3105.5866
   3156.7515   3179.6747   3193.4490


== Thermochemistry energies (hartree) ==
  ZPVE =     0.133006  (after scaling by 0.985)
W1  Ee =  -384.455687  (total electronic energy)
W1  U0 =  -384.322681  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.803165  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.299070   -0.196085   -0.213970
C    -1.655256    1.161478   -0.165435
C    -0.408862    1.347724    0.272420
C     0.416180    0.224073    0.732710
C    -0.094132   -1.062846    0.625645
C    -1.261076   -1.328111   -0.270785
H    -1.724158   -2.287033   -0.035462
H    -0.889539   -1.411158   -1.302161
H     0.436548   -1.891691    1.074707
H     3.135750   -0.968796   -0.441634
H     0.027237    2.336439    0.307418
H    -2.253785    2.013515   -0.465524
H    -2.969641   -0.263827   -1.072610
H    -2.936286   -0.314311    0.671643
O     1.736237    0.255144   -0.649838
H     1.158986    0.430365    1.490083
O     2.992287   -0.070256   -0.113908

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -479.1690     65.6313     94.3683    156.8542    209.4955    262.7825    330.1102
    401.8430    488.7220    494.3236    570.6013    681.8319    737.1496    772.0551
    850.3111    920.4002    943.4608    956.6538    997.3871   1003.3371   1033.2789
   1044.1860   1071.9139   1168.9090   1185.6612   1193.0659   1271.6017   1337.8422
   1362.7851   1366.8863   1407.9550   1441.6654   1464.5955   1479.9433   1489.9663
   1690.4307   2955.4688   2984.0717   3053.4172   3064.1140   3151.9431   3167.8138
   3180.8024   3190.1657   3725.4775


== Thermochemistry energies (hartree) ==
  ZPVE =      0.135585  (after scaling by 0.985)
W1  Ee =  -384.459553  (total electronic energy)
W1  U0 =  -384.323967  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.806844  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -2.223899    0.161868   -0.227947
C    -1.325821    1.361280   -0.090856
C    -0.060527    1.293214    0.310697
C     0.581099    0.000536    0.707352
C    -0.263813   -1.195963    0.550404
C    -1.436726   -1.156505   -0.359892
H    -2.082505   -2.018631   -0.187519
H    -1.074157   -1.243494   -1.390655
H     0.025257   -2.102103    1.059660
H     3.433501   -0.412408   -0.342145
H     0.558310    2.178680    0.366847
H    -1.756256    2.324272   -0.341334
H    -2.869798    0.285222   -1.099595
H    -2.898025    0.109307    0.633967
O     1.386772   -0.605026   -0.275917
H     1.102364    0.078849    1.665261
O     2.855656    0.356741   -0.436963

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -692.9884     77.6399    123.9571    148.2492    171.6387    263.1074    286.3824
    391.8943    491.0862    514.7627    548.4615    682.2424    740.2509    758.9012
    836.1047    890.1370    927.4350    939.2235    982.8791   1003.2165   1012.1423
   1024.6623   1062.7242   1142.6279   1181.0295   1187.5187   1268.6737   1280.3931
   1322.3762   1358.8797   1400.2520   1413.1941   1427.0980   1461.0656   1485.9193
   1711.5802   2994.3368   3004.9032   3021.6573   3051.4205   3065.4767   3144.4631
   3183.3964   3212.2372   3783.4494


== Thermochemistry energies (hartree) ==
  ZPVE =     0.134592  (after scaling by 0.985)
W1  Ee =  -384.460885  (total electronic energy)
W1  U0 =  -384.326292  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.808512  (total electronic energy)
```

Hydrocarbon 8: cyclohexadienyl

Species 1: ·R

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -0.737889    1.221604   -0.000038
C    -1.450248    0.000031   -0.000067
C    -0.737926   -1.221599   -0.000028
C     0.621460   -1.251915    0.000036
C     1.443130   -0.000017    0.000064
C     0.621497    1.251898    0.000024
H     2.130147   -0.000036   -0.862556
H     2.130077   -0.000027    0.862740
H     1.146183   -2.198753    0.000065
H    -1.291116   -2.152801   -0.000050
H    -2.530657    0.000054   -0.000118
H     1.146249    2.198707    0.000045
H    -1.291031    2.152836   -0.000066

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    176.0298    387.1752    530.6199    567.3433    595.0751    637.9271    730.5061
    778.3793    870.6522    937.4595    968.2708    975.7039    981.1546    989.0958
   1002.7897   1111.3566   1172.9426   1181.5453   1200.5367   1308.1508   1375.8194
   1419.3486   1436.2672   1461.7327   1548.2440   1611.6555   2898.3662   2917.0645
   3151.0892   3153.2749   3171.2412   3172.2629   3195.2074


== Thermochemistry energies (hartree) ==
  ZPVE =     0.106846  (after scaling by 0.985)
W1  Ee =  -232.842303  (total electronic energy)
W1  U0 =  -232.735457  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -232.425751  (total electronic energy)
```

Species 2: ROO·

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.956865    0.346859   -0.518726
C     1.645193   -1.028658   -0.148662
C     0.474853   -1.363847    0.407190
C    -0.583171   -0.330359    0.610632
C    -0.050841    1.093203    0.707940
C     1.164037    1.350083   -0.131338
H     0.200104    1.292701    1.757759
H    -0.865296    1.778180    0.465905
H     0.242576   -2.390223    0.654831
H     2.389706   -1.791640   -0.338855
O    -1.490077   -0.452921   -0.583589
H    -1.231379   -0.554826    1.454818
O    -2.589509    0.246342   -0.427325
H     1.406020    2.376141   -0.376396
H     2.853345    0.538614   -1.092958

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     77.5007    123.8378    212.1933    312.2362    379.4636    467.5307    513.7466
    593.3316    613.9147    664.2412    780.2658    803.9229    851.4722    951.8753
    964.5986    976.8052    997.0837   1007.5129   1016.2330   1102.6011   1180.4663
   1181.8199   1209.7835   1222.3361   1321.8164   1340.0181   1369.3630   1417.7412
   1449.1206   1455.5894   1632.3970   1708.5379   2989.5011   3067.7671   3091.3215
   3158.8490   3166.8211   3184.3193   3190.6602


== Thermochemistry energies (hartree) ==
  ZPVE =     0.116124  (after scaling by 0.985)
W1  Ee =  -383.279971  (total electronic energy)
W1  U0 =  -383.163847  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.627788  (total electronic energy)
```

Species 3: ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     2.224674    0.297077   -0.240221
C     1.777279   -1.034396   -0.093365
C     0.488253   -1.316405    0.235847
C    -0.521703   -0.240470    0.461840
C     0.025238    1.140450    0.296675
C     1.322809    1.366364   -0.042275
H    -0.660488    1.961840    0.453300
H     0.143445   -2.336356    0.334018
H     2.477762   -1.845669   -0.245703
O    -1.597659   -0.521667   -0.485234
H    -0.977684   -0.352737    1.455528
O    -2.768974    0.219996   -0.045508
H    -2.876867    0.831415   -0.785842
H     3.251400    0.496563   -0.511848
H     1.676194    2.382593   -0.164520

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
     79.2374    122.2077    233.2789    246.1991    368.3294    384.8999    451.4580
    566.4050    589.2951    620.1657    689.6509    758.9581    820.7487    881.0823
    916.7612    921.0026    980.8896    986.0679    995.0809   1010.7220   1042.5649
   1124.7775   1171.1189   1196.3741   1294.9448   1315.1023   1358.9225   1367.2804
   1420.9243   1457.2428   1548.1899   1599.4366   2947.6646   3158.4139   3163.7171
   3184.6960   3188.5850   3197.0912   3764.0579


== Thermochemistry energies (hartree) ==
  ZPVE =     0.114721  (after scaling by 0.985)
W1  Ee =  -383.290912  (total electronic energy)
W1  U0 =  -383.176191  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.638077  (total electronic energy)
```

Species 4: *cy*-ether

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.433779    0.722586    0.125465
C    -1.433779   -0.722586    0.125465
C    -0.326795   -1.426679   -0.179528
C     0.967023   -0.756897   -0.321931
C     0.967023    0.756897   -0.321931
C    -0.326795    1.426679   -0.179528
H    -0.376011   -2.493879   -0.351591
H    -2.377087   -1.233908    0.267104
O     1.439253   -0.000000    0.797719
H     1.757388   -1.278911   -0.850431
H     1.757389    1.278910   -0.850431
H    -0.376011    2.493879   -0.351591
H    -2.377087    1.233909    0.267104

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    254.5645    319.6290    464.0374    544.0407    617.7931    641.4945    700.2252
    776.4804    778.8320    848.4227    937.1743    978.9011    980.7757    985.0101
    998.5682   1011.0676   1060.3064   1139.2626   1191.0942   1207.9378   1254.7997
   1368.2575   1377.9465   1428.8727   1468.0560   1598.8930   1683.8256   3120.4087
   3128.7354   3158.2146   3167.1955   3179.4352   3187.3396


== Thermochemistry energies (hartree) ==
  ZPVE =     0.102231  (after scaling by 0.985)
W1  Ee =  -307.503749  (total electronic energy)
W1  U0 =  -307.401518  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -306.969394  (total electronic energy)
```

Species 5: alkene

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.204275    0.000000    0.695286
C     0.000000    0.000000    1.390572
C    -1.204275   -0.000000    0.695286
C    -1.204275    0.000000   -0.695286
C     0.000000    0.000000   -1.390572
C     1.204275   -0.000000   -0.695286
H    -0.000000   -0.000000   -2.472631
H    -2.141364   -0.000000    1.236319
H    -0.000000   -0.000000    2.472631
H    -2.141364    0.000000   -1.236319
H     2.141364    0.000000    1.236319
H     2.141364   -0.000000   -1.236319

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
    414.2583    414.2664    624.2435    624.2601    691.3378    726.8158    867.7603
    867.8529    988.7645    988.8385   1015.7570   1022.1306   1030.6246   1062.5109
   1062.5212   1176.7232   1200.5782   1200.6070   1336.0266   1389.9919   1519.1495
   1519.1555   1638.0856   1638.1330   3156.6715   3166.4396   3166.4962   3182.1573
   3182.2164   3192.2781


== Thermochemistry energies (hartree) ==
  ZPVE =     0.098885  (after scaling by 0.985)
W1  Ee =  -232.300335  (total electronic energy)
W1  U0 =  -232.201450  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -231.883433  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     2.039109   -0.170311    0.264779
C     1.459844    1.148259    0.238985
C     0.210315    1.358437   -0.208726
C    -0.663977    0.250077   -0.742509
C    -0.094025   -1.147665   -0.388138
C     1.294520   -1.264931   -0.068494
H    -0.527346   -1.965046   -0.959297
H    -0.821505   -1.095132    0.674189
H    -0.222812    2.350635   -0.217540
H     2.059142    1.982964    0.579788
O    -1.928004    0.251190   -0.233245
H    -0.788689    0.385322   -1.825738
O    -1.821466   -0.272379    1.067373
H     1.746741   -2.248614   -0.051809
H     3.075517   -0.283816    0.551998

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
  -2046.9106     66.3417    191.2526    342.8088    397.4710    486.1543    503.9823
    585.9483    647.1014    661.5381    746.1241    791.7509    827.0686    891.1354
    933.3106    974.1660    980.6267    989.1944   1008.3676   1034.0094   1099.7406
   1165.1320   1178.2550   1198.5344   1244.5535   1278.5771   1354.4702   1371.4373
   1422.8318   1475.1149   1512.5722   1649.2854   1732.9508   2968.6544   3110.8531
   3158.3046   3165.1891   3178.3776   3190.1904


== Thermochemistry energies (hartree) ==
  ZPVE =     0.111108  (after scaling by 0.985)
W1  Ee =  -383.230050  (total electronic energy)
W1  U0 =  -383.118942  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.577607  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C    -1.916263   -0.540440   -0.585835
C    -1.743770    0.865041   -0.493914
C    -0.738017    1.405880    0.288329
C     0.154272    0.581742    0.960337
C     0.075390   -0.871782    0.825275
C    -1.080725   -1.381086    0.076909
H     0.282558   -1.420148    1.748245
H     1.030694   -1.132813    0.206047
H    -0.652106    2.479456    0.388828
H    -2.429195    1.518692   -1.016262
O     2.179351    0.649136   -0.441894
H     0.859653    1.004142    1.658652
O     2.366327   -0.576291   -0.591716
H    -1.225218   -2.452312    0.025982
H    -2.737132   -0.935910   -1.169208

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -329.8489     77.4220    111.1944    123.1083    236.6692    374.8175    432.6514
    582.8818    592.9938    605.4823    687.3251    799.9340    829.5936    894.2920
    926.9943    981.3280    999.5739   1005.8484   1015.4647   1019.3672   1111.3980
   1163.8324   1183.9519   1205.3364   1341.1150   1356.6363   1377.5680   1406.7579
   1459.2391   1483.3767   1544.1480   1620.2798   2047.3851   3035.6460   3164.0595
   3172.3181   3182.2871   3191.7973   3212.6344


== Thermochemistry energies (hartree) ==
  ZPVE =     0.111205  (after scaling by 0.985)
W1  Ee =  -383.255832  (total electronic energy)
W1  U0 =  -383.144627  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.604858  (total electronic energy)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     2.125538    0.317637   -0.439337
C     1.753148   -1.013855   -0.192889
C     0.551413   -1.304265    0.400823
C    -0.388931   -0.257113    0.701808
C     0.071230    1.096344    0.545220
C     1.280295    1.364514   -0.051183
H    -0.575937    1.902832    0.862965
H     0.265764   -2.327483    0.600119
H     2.431758   -1.814259   -0.457002
O    -1.608256   -0.477850   -0.596988
H    -1.107861   -0.448549    1.487497
O    -2.802062    0.170289   -0.210945
H    -2.752171    1.004793   -0.697993
H     3.074573    0.534362   -0.910113
H     1.590261    2.389220   -0.208657

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -560.2710     63.9930    121.1052    178.6775    321.9084    383.9804    405.0602
    421.8122    604.0396    607.5185    654.1512    721.0996    810.5345    881.2507
    918.7992    952.3258    981.7518    995.4800   1020.9738   1023.2535   1050.5258
   1103.8248   1165.2621   1176.3980   1198.5862   1326.6038   1364.9434   1381.5530
   1478.2204   1487.3568   1558.1038   1597.8141   3152.7484   3164.1465   3169.4935
   3181.9021   3189.5294   3196.1885   3723.3766


== Thermochemistry energies (hartree) ==
  ZPVE =     0.113847  (after scaling by 0.985)
W1  Ee =  -383.274905  (total electronic energy)
W1  U0 =  -383.161057  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.622302  (total electronic energy)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ W1 data ]

== B3LYP/cc-pVTZ+d equilibrium geometry (Angstrom) ==
C     1.971223    0.271571   -0.534941
C     1.599369   -1.020813   -0.254460
C     0.423075   -1.278747    0.463847
C    -0.501938   -0.168307    0.813278
C     0.055888    1.201676    0.619782
C     1.200782    1.387301   -0.067711
H    -0.498646    2.036417    1.024495
H     0.153516   -2.276369    0.769331
H     2.222843   -1.848009   -0.565452
O    -1.163651   -0.700903   -0.310159
H    -1.080550   -0.281396    1.730889
O    -2.733639    0.295262   -0.493029
H    -2.567442    0.412720   -1.438848
H     2.881688    0.459266   -1.088300
H     1.576515    2.386413   -0.245391

== B3LYP/cc-pVTZ+d harmonic frequencies (cm^-1) ==
   -686.0759     72.5454    130.9785    169.8612    211.1387    296.3470    357.7189
    451.5503    574.5507    587.7637    622.9115    733.6244    779.9857    808.7352
    858.0155    910.7056    946.1703    972.8360    992.2048    998.1940   1003.4736
   1046.5849   1147.8120   1181.8960   1191.5369   1271.1764   1335.9466   1376.7738
   1432.4006   1474.9238   1521.7076   1641.6560   3053.1215   3165.0514   3174.8370
   3189.0533   3197.5062   3228.6068   3776.5610


== Thermochemistry energies (hartree) ==
  ZPVE =     0.111945  (after scaling by 0.985)
W1  Ee =  -383.252212  (total electronic energy)
W1  U0 =  -383.140267  (Zero-kelvin internal energy)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -382.600630  (total electronic energy)
```

G4-level equilibrium geometry, harmonic frequencies, and thermochemistry energies of different reaction species involved in combustion reaction of R·

Hydrocarbon 1: ethyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.693143    0.000000   -0.001240
C     0.794299    0.000000   -0.022046
H    -1.108801    0.886739   -0.492488
H    -1.094054   -0.000000    1.027312
H    -1.108801   -0.886739   -0.492489
H     1.352360    0.926401    0.048693
H     1.352360   -0.926401    0.048693

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    118.5220    463.2274    806.8069    979.8948   1066.5708   1193.8214   1398.5265
   1465.2600   1480.2369   1482.7358   2955.0694   3046.5395   3091.9310   3153.5073
   3255.0012

== Thermochemistry energies (hartree) ==
  ZPVE =     0.058272  (after scaling by 0.9854)
G4  Ee =  -79.137363  (total electronic energy)
G4  U0 =  -79.079091  (Zero-kelvin internal energy)
G4  UT =  -79.075101  (Internal energy at 298.15 K)
G4  HT =  -79.074156  (Enthalpy at 298.15 K)
G4  GT =  -79.103260  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.460888   -0.473836   -0.092055
C    -0.493664    0.643320    0.254520
O     0.800895    0.431569   -0.382490
O     1.445587   -0.567942    0.176034
H    -0.817619    1.613124   -0.133159
H    -0.314809    0.716925    1.330408
H    -1.623000   -0.530237   -1.172004
H    -2.424507   -0.295566    0.394600
H    -1.064599   -1.430171    0.257011

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    112.7331    232.0360    356.3188    529.4444    797.2629    846.9625    997.8804
   1095.8060   1165.9238   1210.3515   1304.5556   1376.3033   1402.9253   1478.4773
   1484.6873   1504.6226   3048.7460   3063.7662   3114.8992   3124.1377   3141.8747


== Thermochemistry energies (hartree) ==
  ZPVE =     0.070467  (after scaling by 0.9854)
G4  Ee =  -229.481519  (total electronic energy)
G4  U0 =  -229.411052  (Zero-kelvin internal energy)
G4  UT =  -229.406119  (Internal energy at 298.15 K)
G4  HT =  -229.405174  (Enthalpy at 298.15 K)
G4  GT =  -229.439050  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.618599    0.608241    0.241659
C    -1.490274   -0.547844   -0.094736
H    -1.564984   -0.881131   -1.124588
H    -2.119073   -1.019689    0.650067
O     0.661371    0.560810   -0.390321
O     1.414366   -0.498673    0.238906
H     1.256291   -1.232272   -0.372965
H    -1.030847    1.554125   -0.148258
H    -0.494049    0.719487    1.325535

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    135.3819    165.1868    223.3654    361.7345    460.2875    554.8496    842.0311
    875.8268    969.3219   1063.6274   1134.5250   1268.6266   1374.6405   1385.1893
   1444.4081   1457.2336   2972.5159   3052.0586   3150.6338   3262.7659   3742.8909


== Thermochemistry energies (hartree) ==
  ZPVE =     0.067116  (after scaling by 0.9854)
G4  Ee =  -229.451560  (total electronic energy)
G4  U0 =  -229.384444  (Zero-kelvin internal energy)
G4  UT =  -229.378707  (Internal energy at 298.15 K)
G4  HT =  -229.377763  (Enthalpy at 298.15 K)
G4  GT =  -229.413034  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.000000    0.733527   -0.370055
C    -0.000000   -0.733527   -0.370055
O    -0.000000    0.000000    0.852095
H    -0.919578    1.272148   -0.594025
H     0.919578    1.272148   -0.594025
H     0.919578   -1.272148   -0.594025
H    -0.919578   -1.272148   -0.594025

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    812.9487    860.5296    901.7281   1044.5186   1154.2404   1154.9537   1170.7754
   1174.4229   1309.2903   1506.7219   1541.9277   3081.6501   3089.8344   3162.4536
   3179.2708

== Thermochemistry energies (hartree) ==
  ZPVE =     0.056449  (after scaling by 0.9854)
G4  Ee =  -153.756763  (total electronic energy)
G4  U0 =  -153.700314  (Zero-kelvin internal energy)
G4  UT =  -153.697144  (Internal energy at 298.15 K)
G4  HT =  -153.696200  (Enthalpy at 298.15 K)
G4  GT =  -153.723745  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.000000   -0.000000    0.663578
C     0.000000   -0.000000   -0.663578
H     0.000000    0.921267    1.238128
H    -0.000000   -0.921267    1.238128
H     0.000000    0.921267   -1.238128
H    -0.000000   -0.921267   -1.238128

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    823.8985    969.0948    982.7256   1072.5933   1237.0082   1386.1028   1472.2881
   1698.8344   3137.7312   3154.3060   3209.3526   3237.0483

== Thermochemistry energies (hartree) ==
  ZPVE =     0.050243  (after scaling by 0.9854)
G4  Ee =  -78.572119  (total electronic energy)
G4  U0 =  -78.521876  (Zero-kelvin internal energy)
G4  UT =  -78.518821  (Internal energy at 298.15 K)
G4  HT =  -78.517876  (Enthalpy at 298.15 K)
G4  GT =  -78.542748  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.227675   -0.564156   -0.119316
C    -0.534338    0.754699    0.211607
O     0.792905    0.591413   -0.292596
O     1.138219   -0.699763    0.162298
H    -0.952597    1.632973   -0.292179
H    -0.523293    0.915949    1.296880
H    -1.477253   -0.732513   -1.166762
H    -1.955102   -0.957857    0.586972
H     0.031331   -1.135005    0.063733

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2268.5031    273.2460    434.8931    552.9337    688.6682    869.5936    904.5487
    919.4689    968.8485   1043.8970   1102.8011   1166.5293   1244.6710   1344.4836
   1452.9097   1495.3830   1746.0743   3023.0273   3082.9184   3108.6442   3203.8479


== Thermochemistry energies (hartree) ==
  ZPVE =     0.064266  (after scaling by 0.9854)
G4  Ee =  -229.416085  (total electronic energy)
G4  U0 =  -229.351819  (Zero-kelvin internal energy)
G4  UT =  -229.347595  (Internal energy at 298.15 K)
G4  HT =  -229.346651  (Enthalpy at 298.15 K)
G4  GT =  -229.378776  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.290788   -0.614114   -0.000044
C     1.037720    0.746214    0.000030
O    -1.145793    0.612125   -0.000036
O    -1.257086   -0.651477    0.000020
H     1.012855    1.323058    0.916843
H     1.012801    1.323117   -0.916744
H     1.634764   -1.086387    0.917859
H     1.634769   -1.086394   -0.917930
H    -0.043207   -0.951173    0.000186

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1069.5196    217.7651    367.9202    477.6298    522.8807    637.6299    823.8097
    898.7402   1010.4460   1036.0826   1223.7203   1288.6078   1325.3064   1363.5363
   1468.6440   1572.9906   1620.0352   3113.8765   3170.5876   3192.4683   3258.3626


== Thermochemistry energies (hartree) ==
  ZPVE =     0.064184  (after scaling by 0.9854)
G4  Ee =  -229.424654  (total electronic energy)
G4  U0 =  -229.360470  (Zero-kelvin internal energy)
G4  UT =  -229.355880  (Internal energy at 298.15 K)
G4  HT =  -229.354936  (Enthalpy at 298.15 K)
G4  GT =  -229.387950  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.923409   -0.549628    0.362510
C     1.632527    0.530041   -0.116358
H     2.190170    0.472496   -1.044352
H     1.569903    1.502348    0.360289
O    -0.771544   -0.467891   -0.483270
O    -1.613328    0.349542    0.252655
H    -1.653877    1.157799   -0.281524
H     1.123553   -1.540209   -0.032105
H     0.513615   -0.528120    1.365702

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -535.3847     89.8197    225.1290    305.8350    420.4425    474.4903    808.9607
    824.5738    936.9307   1032.4690   1085.1118   1238.2991   1270.6563   1403.3411
   1464.7228   1543.8180   3149.7743   3155.1357   3228.2447   3254.1159   3701.6005


== Thermochemistry energies (hartree) ==
  ZPVE =     0.066479  (after scaling by 0.9854)
G4  Ee =  -229.422775  (total electronic energy)
G4  U0 =  -229.356296  (Zero-kelvin internal energy)
G4  UT =  -229.350902  (Internal energy at 298.15 K)
G4  HT =  -229.349958  (Enthalpy at 298.15 K)
G4  GT =  -229.384909  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.578363    0.709482    0.033643
C    -1.688552   -0.261274    0.040263
H    -2.118764   -0.609603   -0.889217
H    -1.987685   -0.738162    0.964049
O     0.197069   -0.440314   -0.122778
O     1.872417    0.025436   -0.038128
H     2.093242   -0.658995    0.610196
H    -0.536914    1.397687   -0.817621
H    -0.404271    1.238849    0.976410

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -776.0281     96.6467    154.2865    257.9157    401.6792    503.9195    759.0851
    829.9545    947.1085   1005.9751   1170.9968   1171.9054   1195.2033   1315.1484
   1465.6598   1534.2704   3030.1281   3084.2994   3177.1143   3295.3648   3779.0766


== Thermochemistry energies (hartree) ==
  ZPVE =     0.065497  (after scaling by 0.9854)
G4  Ee =  -229.423786  (total electronic energy)
G4  U0 =  -229.358289  (Zero-kelvin internal energy)
G4  UT =  -229.352718  (Internal energy at 298.15 K)
G4  HT =  -229.351774  (Enthalpy at 298.15 K)
G4  GT =  -229.386942  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 2: isopropyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.011385   -0.196921   -1.299512
C    -0.011385    0.533303    0.000000
C    -0.011385   -0.196921    1.299512
H    -0.267671    0.457984   -2.138299
H    -0.721788   -1.034156   -1.291916
H     0.974708   -0.637805   -1.531680
H     0.234440    1.591182    0.000000
H    -0.721788   -1.034156    1.291916
H    -0.267671    0.457984    2.138299
H     0.974708   -0.637805    1.531680

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    114.2539    122.5276    360.2223    412.3982    883.1156    936.3367    941.7395
   1034.0765   1151.1549   1177.4816   1367.5720   1405.3871   1412.5419   1468.9112
   1479.5068   1479.7926   1490.5800   2942.1611   2947.3639   3029.7343   3031.5121
   3090.9189   3091.5475   3170.1558

== Thermochemistry energies (hartree) ==
  ZPVE =     0.086521  (after scaling by 0.9854)
G4  Ee =  -118.447899  (total electronic energy)
G4  U0 =  -118.361378  (Zero-kelvin internal energy)
G4  UT =  -118.356198  (Internal energy at 298.15 K)
G4  HT =  -118.355253  (Enthalpy at 298.15 K)
G4  GT =  -118.388585  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.577658   -0.823329    0.024841
C     0.367361    0.019925   -0.340583
C     0.447706    1.470383    0.109891
H     1.442063   -1.860998   -0.290845
H     1.748408   -0.808158    1.105591
H     2.469025   -0.425444   -0.468061
H     0.647817    1.532825    1.184150
H    -0.494117    1.979411   -0.105738
H     1.253346    1.984335   -0.422934
O    -0.775775   -0.630913    0.322022
O    -1.921246   -0.164938   -0.116342
H     0.153281   -0.037041   -1.412495

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    102.4036    196.0301    237.7539    299.7051    338.2530    447.9377    524.2669
    797.0390    889.5823    933.5030    948.7715   1124.9089   1157.2540   1196.8417
   1221.9526   1341.8293   1362.0283   1397.1737   1415.8216   1480.0608   1485.8040
   1491.4014   1509.4188   3043.3012   3047.4302   3064.5749   3114.7198   3123.6286
   3126.4236   3136.5185

== Thermochemistry energies (hartree) ==
  ZPVE =     0.097780  (after scaling by 0.9854)
G4  Ee =  -268.794777  (total electronic energy)
G4  U0 =  -268.696997  (Zero-kelvin internal energy)
G4  UT =  -268.690685  (Internal energy at 298.15 K)
G4  HT =  -268.689741  (Enthalpy at 298.15 K)
G4  GT =  -268.727007  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.696364   -0.680072   -0.028858
C    -0.408347    0.070213    0.335817
C    -0.414776    1.492985   -0.110307
H    -1.624419   -1.724710    0.286493
H    -1.864612   -0.649910   -1.109193
H    -2.551959   -0.216094    0.468199
H    -0.430855    1.717136   -1.172597
H    -0.483695    2.313093    0.593575
O     0.625862   -0.685257   -0.318260
O     1.898033   -0.215453    0.171505
H    -0.240425    0.012621    1.418388
H     2.121728    0.454786   -0.490748

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    107.6434    141.1428    214.9469    227.7827    283.1771    328.9959    456.3603
    477.1515    564.4452    837.2918    909.9851    923.8900    961.0398   1041.1470
   1154.9425   1172.7448   1313.0969   1376.5472   1388.3862   1391.6242   1453.0799
   1481.2488   1494.9350   3031.9261   3044.5794   3122.9781   3127.8782   3143.9956
   3258.0072   3738.2843

== Thermochemistry energies (hartree) ==
  ZPVE =     0.094666  (after scaling by 0.9854)
G4  Ee =  -268.764214  (total electronic energy)
G4  U0 =  -268.669548  (Zero-kelvin internal energy)
G4  UT =  -268.662376  (Internal energy at 298.15 K)
G4  HT =  -268.661432  (Enthalpy at 298.15 K)
G4  GT =  -268.700288  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.509832    0.101084   -0.147961
C    -0.151286   -0.041127    0.486983
C     1.044170    0.613579   -0.058565
H    -2.082614   -0.826798   -0.048580
H    -1.415537    0.332323   -1.212510
H    -2.079920    0.901623    0.335837
O     0.825822   -0.785995   -0.244382
H    -0.154967   -0.260138    1.556434
H     1.872069    0.876681    0.598688
H     0.956081    1.223054   -0.957555

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    207.1293    363.3563    405.8293    780.2022    854.3706    903.7468    979.6860
   1040.9844   1131.9713   1157.6617   1164.1154   1186.5905   1298.6872   1403.2619
   1439.6703   1483.3858   1497.2284   1532.7950   3035.5031   3078.3983   3089.2485
   3100.5687   3122.1771   3164.2167

== Thermochemistry energies (hartree) ==
  ZPVE =     0.084006  (after scaling by 0.9854)
G4  Ee =  -193.070090  (total electronic energy)
G4  U0 =  -192.986084  (Zero-kelvin internal energy)
G4  UT =  -192.981621  (Internal energy at 298.15 K)
G4  HT =  -192.980677  (Enthalpy at 298.15 K)
G4  GT =  -193.012495  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.232927    0.162649    0.000086
C     0.134410   -0.453581    0.000057
C     1.280713    0.219347   -0.000150
H    -1.809402   -0.152027    0.878917
H    -1.809585   -0.152340   -0.878513
H    -1.181336    1.255270   -0.000113
H     0.161772   -1.542820    0.000228
H     1.303924    1.305847   -0.000325
H     2.241453   -0.284420   -0.000152

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    211.5706    420.7874    591.4733    927.6020    943.8587    944.2965   1036.3900
   1071.3711   1190.1796   1329.1228   1406.0328   1451.1097   1480.0638   1494.0332
   1722.1810   3019.8062   3067.5182   3105.2242   3133.7390   3143.3223   3223.0458


== Thermochemistry energies (hartree) ==
  ZPVE =     0.078376  (after scaling by 0.9854)
G4  Ee =  -117.882262  (total electronic energy)
G4  U0 =  -117.803886  (Zero-kelvin internal energy)
G4  UT =  -117.799772  (Internal energy at 298.15 K)
G4  HT =  -117.798828  (Enthalpy at 298.15 K)
G4  GT =  -117.828901  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.110278    1.384917   -0.117585
H     0.041313    2.239980    0.551660
H    -0.077387    1.617650   -1.166837
H     1.369421    0.803521   -0.078050
C    -0.414000    0.033077    0.374410
H    -0.335241    0.002801    1.470014
C    -1.813372   -0.343923   -0.083640
H    -2.544892    0.357336    0.327988
H    -1.879922   -0.320818   -1.174824
H    -2.071546   -1.349336    0.261788
O     1.766942   -0.313214    0.037975
O     0.508161   -0.911232   -0.191831

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2226.9706    191.2786    203.7125    313.6092    395.0579    481.5921    567.5939
    657.6417    844.9281    877.0044    928.5725    958.7633    970.6661   1091.4146
   1105.9478   1138.3719   1179.5933   1335.0816   1369.8462   1404.5544   1454.2401
   1482.1446   1494.0665   1740.6918   3011.0370   3044.1964   3098.0688   3118.7939
   3125.5754   3195.9261

== Thermochemistry energies (hartree) ==
  ZPVE =     0.091547  (after scaling by 0.9854)
G4  Ee =  -268.730305  (total electronic energy)
G4  U0 =  -268.638758  (Zero-kelvin internal energy)
G4  UT =  -268.633080  (Internal energy at 298.15 K)
G4  HT =  -268.632136  (Enthalpy at 298.15 K)
G4  GT =  -268.667813  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.314241    1.410888   -0.046247
H    -0.063688    2.222794    0.633463
H    -0.652831    1.723090   -1.033368
H     0.929825    0.901967   -0.309579
C    -0.814911    0.228792    0.479796
H    -0.747221    0.061870    1.550797
C    -1.667453   -0.734115   -0.282225
H    -1.544439   -0.611474   -1.361872
H    -1.444029   -1.770510   -0.016120
H    -2.725608   -0.555730   -0.044981
O     1.789392   -0.007605   -0.293847
O     1.089061   -0.918069    0.253061

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1056.5180    149.9273    177.3243    211.1493    377.5832    417.1416    513.8589
    624.1585    628.8354    897.4681    951.0000    961.8331   1034.7590   1059.8253
   1195.6700   1278.2385   1304.7990   1349.5525   1402.0639   1440.7209   1476.0572
   1486.7957   1577.1925   1621.3695   3017.4827   3086.4144   3105.1864   3123.7467
   3172.5121   3193.1341

== Thermochemistry energies (hartree) ==
  ZPVE =     0.091673  (after scaling by 0.9854)
G4  Ee =  -268.738372  (total electronic energy)
G4  U0 =  -268.646699  (Zero-kelvin internal energy)
G4  UT =  -268.640611  (Internal energy at 298.15 K)
G4  HT =  -268.639667  (Enthalpy at 298.15 K)
G4  GT =  -268.676490  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.728444    1.458539   -0.117607
H    -0.140880    2.268476    0.299235
H    -1.280245    1.662274   -1.029457
H     2.422997    0.497621   -0.345665
C    -0.665769    0.180822    0.405969
H    -0.228396    0.064131    1.393361
C    -1.642664   -0.888256   -0.001393
H    -1.972902   -0.750369   -1.035017
H    -1.189857   -1.877724    0.092842
H    -2.528473   -0.854483    0.643339
O     2.016007   -0.158115    0.240685
O     0.876370   -0.531455   -0.458241

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -510.6325     73.9664    148.4748    199.5973    296.0618    317.6227    420.4921
    437.7855    524.8368    800.9840    898.3091    939.1007    971.4038   1024.7257
   1082.6882   1190.3001   1269.8738   1393.2870   1400.6964   1430.5409   1478.0532
   1494.0238   1532.5534   3036.9470   3100.9146   3128.7399   3148.3231   3167.0458
   3243.5192   3707.6151

== Thermochemistry energies (hartree) ==
  ZPVE =     0.093968  (after scaling by 0.9854)
G4  Ee =  -268.735844  (total electronic energy)
G4  U0 =  -268.641876  (Zero-kelvin internal energy)
G4  UT =  -268.635051  (Internal energy at 298.15 K)
G4  HT =  -268.634107  (Enthalpy at 298.15 K)
G4  GT =  -268.672728  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.338345   -1.100022   -0.021549
H     1.366409   -2.013474    0.557365
H     1.815025   -1.082327   -0.993683
C     0.508811    0.042643    0.417080
H     0.307695    0.047376    1.495743
C     0.840580    1.427764   -0.101137
H     1.066238    1.393359   -1.171051
H    -0.018164    2.086070    0.050890
H     1.701596    1.844220    0.431870
O    -0.488894   -0.633614   -0.300943
O    -2.002545    0.153594   -0.003931
H    -2.433703   -0.657381    0.301502

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -763.2279    107.2972    158.7234    205.2157    250.7445    348.0349    411.5111
    426.4045    538.9001    749.8319    848.2850    913.1887    922.5303    988.8375
   1092.8574   1165.8846   1198.6501   1288.8660   1390.2481   1419.8835   1462.8959
   1485.5992   1496.9920   3027.1544   3041.2437   3114.9221   3131.6148   3169.2382
   3288.1386   3781.9958

== Thermochemistry energies (hartree) ==
  ZPVE =     0.092997  (after scaling by 0.9854)
G4  Ee =  -268.739354  (total electronic energy)
G4  U0 =  -268.646357  (Zero-kelvin internal energy)
G4  UT =  -268.639529  (Internal energy at 298.15 K)
G4  HT =  -268.638585  (Enthalpy at 298.15 K)
G4  GT =  -268.676843  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 3: isobutyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.270846   -0.680363    0.102063
C    -0.000002    0.059666   -0.349082
C    -0.000016    1.482759    0.102670
C     1.270861   -0.680336    0.102047
H    -2.172669   -0.165652   -0.245162
H    -1.318699   -0.738652    1.194985
H    -1.292874   -1.701416   -0.292503
H    -0.928251    2.035950    0.197606
H     0.928219    2.035916    0.197795
H    -0.000013    0.049111   -1.456180
H     1.318736   -0.738609    1.194970
H     2.172669   -0.165616   -0.245203
H     1.292897   -1.701395   -0.292503

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    117.8511    227.6033    253.6171    355.4117    368.4169    398.6169    517.3034
    813.0107    902.6052    942.4934    967.6414    983.6116   1090.5173   1180.5211
   1205.2915   1316.6458   1328.9030   1395.7230   1411.9473   1463.8186   1487.4612
   1491.4249   1501.7841   1510.6137   2901.0422   3026.5851   3030.5512   3096.3871
   3099.0995   3099.9571   3102.2564   3141.2584   3244.0392

== Thermochemistry energies (hartree) ==
  ZPVE =     0.114432  (after scaling by 0.9854)
G4  Ee =  -157.752204  (total electronic energy)
G4  U0 =  -157.637772  (Zero-kelvin internal energy)
G4  UT =  -157.631585  (Internal energy at 298.15 K)
G4  HT =  -157.630641  (Enthalpy at 298.15 K)
G4  GT =  -157.666572  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.993447   -0.884283   -0.174053
C     0.736607   -0.011677   -0.285763
C    -0.358784   -0.575291    0.617560
C     1.032218    1.458422    0.034614
H     1.787957   -1.926218   -0.440640
H     2.396816   -0.870776    0.845476
H     2.777287   -0.515647   -0.842478
H     0.351817   -0.080389   -1.310841
H     1.435417    1.565572    1.048885
H     0.128652    2.069818   -0.035320
H     1.772029    1.865070   -0.661593
O    -1.613844    0.146458    0.459699
O    -2.184925   -0.140240   -0.689515
H    -0.117504   -0.452699    1.678828
H    -0.563253   -1.627504    0.402056

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     76.6961    112.5276    218.5098    233.7486    250.3893    330.3757    412.2006
    413.0510    568.5512    818.7657    876.7285    934.2737    947.0305    957.8638
    976.3325   1141.3825   1167.6864   1196.7295   1205.5467   1287.1245   1321.6878
   1372.2193   1383.5363   1402.2594   1423.5858   1472.0624   1488.7217   1494.1276
   1504.7754   1510.8486   3026.9395   3029.6620   3036.7481   3052.5211   3092.3866
   3098.2143   3106.7795   3115.2595   3118.7428

== Thermochemistry energies (hartree) ==
  ZPVE =     0.126111  (after scaling by 0.9854)
G4  Ee =  -308.097564  (total electronic energy)
G4  U0 =  -307.971453  (Zero-kelvin internal energy)
G4  UT =  -307.963915  (Internal energy at 298.15 K)
G4  HT =  -307.962971  (Enthalpy at 298.15 K)
G4  GT =  -308.003593  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.831619   -1.059756   -0.241913
C     0.822321   -0.006088    0.073372
C    -0.382699   -0.329430    0.898202
C     1.152604    1.431104   -0.177911
H     1.395311   -2.063328   -0.217651
H     2.674053   -1.056922    0.471694
H     2.279490   -0.904878   -1.232392
H     1.906122    1.808716    0.535002
H     0.267249    2.066115   -0.079374
H     1.580374    1.582529   -1.177104
O    -1.585177    0.289429    0.428723
O    -1.949948   -0.356725   -0.810002
H    -0.308569    0.084026    1.919174
H    -0.534991   -1.412395    0.980030
H    -1.521104    0.219519   -1.459636

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     46.5844     83.9263    116.0644    141.0837    200.4833    244.8936    308.0653
    359.6478    399.5900    556.7743    775.8179    870.8506    941.2752    945.8924
    971.8560   1002.4326   1016.4325   1056.8573   1241.5226   1290.7011   1303.0402
   1376.7427   1384.5439   1397.6612   1414.1249   1454.6200   1468.2357   1474.7994
   1486.0105   1495.4335   2952.7097   2955.8001   2962.0161   3029.3251   3037.3015
   3050.2585   3094.0948   3103.3924   3737.2827

== Thermochemistry energies (hartree) ==
  ZPVE =     0.122904  (after scaling by 0.9854)
G4  Ee =  -308.075988  (total electronic energy)
G4  U0 =  -307.953084  (Zero-kelvin internal energy)
G4  UT =  -307.944426  (Internal energy at 298.15 K)
G4  HT =  -307.943482  (Enthalpy at 298.15 K)
G4  GT =  -307.987137  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.052805    0.932113    1.283142
C    -0.052805    0.130594    0.000000
C    -0.576412   -1.243896   -0.000000
C    -0.052805    0.932113   -1.283142
H    -0.017656    0.271445    2.152650
H    -0.950137    1.556461    1.353379
H     0.818908    1.594574    1.321459
H    -0.950137    1.556461   -1.353379
H    -0.017656    0.271445   -2.152650
H     0.818908    1.594574   -1.321459
O     0.832730   -1.000942   -0.000000
H    -0.977554   -1.671483   -0.918593
H    -0.977554   -1.671483    0.918593

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    179.6030    217.1014    350.5030    358.3323    406.1078    408.5472    704.3365
    819.1405    904.8970    931.7381    955.3221   1017.9411   1076.7892   1134.1790
   1149.2917   1173.5645   1282.5037   1394.2902   1409.6260   1421.4209   1473.7738
   1485.9881   1493.5316   1505.9467   1536.4685   3031.3025   3036.3834   3074.7740
   3093.4869   3098.3991   3122.4915   3124.6722   3158.3729

== Thermochemistry energies (hartree) ==
  ZPVE =     0.111192  (after scaling by 0.9854)
G4  Ee =  -232.384120  (total electronic energy)
G4  U0 =  -232.272928  (Zero-kelvin internal energy)
G4  UT =  -232.267081  (Internal energy at 298.15 K)
G4  HT =  -232.266137  (Enthalpy at 298.15 K)
G4  GT =  -232.301294  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.274947   -0.677941    0.000003
C     0.000000    0.124566   -0.000002
C     0.000001    1.456978   -0.000016
C    -1.274949   -0.677939    0.000011
H     2.159636   -0.036470   -0.000009
H     1.327183   -1.334165   -0.878355
H     1.327191   -1.334143    0.878378
H    -1.327192   -1.334163   -0.878347
H    -2.159636   -0.036467    0.000006
H    -1.327187   -1.334141    0.878386
H     0.923232    2.027782   -0.000025
H    -0.923229    2.027784   -0.000019

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    176.6651    213.5577    376.2478    435.0083    442.6857    708.8943    817.1783
    927.1980    962.8198    987.0313   1023.8777   1087.9719   1107.6406   1295.7868
   1407.9467   1413.5192   1448.0732   1470.7393   1483.9391   1488.7150   1503.0376
   1729.3903   3013.1169   3018.9421   3059.9435   3063.1561   3114.0538   3116.0626
   3141.8320   3220.9491

== Thermochemistry energies (hartree) ==
  ZPVE =     0.106085  (after scaling by 0.9854)
G4  Ee =  -157.194053  (total electronic energy)
G4  U0 =  -157.087968  (Zero-kelvin internal energy)
G4  UT =  -157.082615  (Internal energy at 298.15 K)
G4  HT =  -157.081671  (Enthalpy at 298.15 K)
G4  GT =  -157.115288  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.750055   -1.012434   -0.150784
C     0.634926   -0.007462   -0.036193
C    -0.497595   -0.322259    0.961210
C     1.027162    1.449398   -0.106941
H     1.366968   -2.034401   -0.232848
H     2.403852   -0.977024    0.734530
H     2.384051   -0.806197   -1.019250
H    -0.315075   -0.199469   -0.986043
H     1.643846    1.724785    0.762485
H     0.142498    2.091895   -0.104984
H     1.618383    1.663787   -1.002580
O    -1.668946    0.189290    0.335786
O    -1.549698   -0.300080   -0.985186
H    -0.406805    0.186608    1.928416
H    -0.575856   -1.407121    1.111720

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2094.7790    130.9551    187.0857    222.6045    258.4590    279.3323    358.5218
    400.2419    548.8562    663.1771    815.3251    914.0868    930.5995    948.3373
    969.0100    982.2558   1015.8978   1121.3007   1134.6814   1227.5586   1252.3396
   1279.5501   1349.5924   1394.7281   1408.9409   1469.4682   1474.4322   1487.9111
   1490.4486   1495.9341   1737.9978   2991.4160   2996.3372   3011.0832   3067.1014
   3072.6199   3076.4448   3107.4691   3120.4451

== Thermochemistry energies (hartree) ==
  ZPVE =     0.119861  (after scaling by 0.9854)
G4  Ee =  -308.042287  (total electronic energy)
G4  U0 =  -307.922426  (Zero-kelvin internal energy)
G4  UT =  -307.915363  (Internal energy at 298.15 K)
G4  HT =  -307.914419  (Enthalpy at 298.15 K)
G4  GT =  -307.953520  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.115711   -0.000014    1.258184
H     0.384200    0.918358    1.767052
H     0.384194   -0.918398    1.767034
C    -0.704316   -0.000001    0.132987
H     0.347260   -0.000002   -0.678183
C    -1.428637    1.288139   -0.255612
H    -1.611592    1.332325   -1.334249
H    -2.403957    1.353066    0.241819
H    -0.848593    2.172747    0.022869
C    -1.428653   -1.288126   -0.255631
H    -1.611611   -1.332293   -1.334268
H    -0.848617   -2.172745    0.022834
H    -2.403972   -1.353051    0.241802
O     2.047017   -0.000005    0.220145
O     1.613990    0.000006   -0.969680

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -950.6294    119.7196    180.4092    192.5747    207.7188    253.0803    364.0117
    381.1310    413.4499    550.6950    674.2667    763.3960    844.6197    944.6406
    968.2937    990.5986   1018.4501   1074.6805   1131.1452   1203.5498   1284.0201
   1358.8595   1404.8451   1413.1960   1422.6891   1479.8161   1492.6723   1496.3667
   1506.1855   1581.8663   1595.6181   3023.6967   3027.2550   3084.4242   3085.9598
   3108.9058   3110.4416   3161.7787   3249.9752

== Thermochemistry energies (hartree) ==
  ZPVE =     0.119350  (after scaling by 0.9854)
G4  Ee =  -308.040364  (total electronic energy)
G4  U0 =  -307.921014  (Zero-kelvin internal energy)
G4  UT =  -307.913479  (Internal energy at 298.15 K)
G4  HT =  -307.912535  (Enthalpy at 298.15 K)
G4  GT =  -307.952736  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.067543   -0.566426    0.992406
H     0.625698    0.036072    1.699395
H     0.039604   -1.630210    1.204593
C    -0.943878    0.006199    0.247711
H     1.911568    0.789152   -1.177612
C    -1.047901    1.494681    0.098807
H    -0.893896    1.800786   -0.946845
H    -2.050512    1.852963    0.369894
H    -0.315438    2.019865    0.715708
C    -1.888834   -0.827839   -0.564770
H    -1.752938   -0.649798   -1.640966
H    -1.752338   -1.896428   -0.382007
H    -2.933505   -0.570818   -0.343081
O     1.547220   -0.760972   -0.205042
O     2.202803    0.462063   -0.312959

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -503.5521     57.1086     96.4916    117.4642    129.9719    173.0104    296.8305
    370.7338    419.0716    436.3775    454.0490    802.2964    874.7200    940.6463
    964.2687    982.7503   1031.8056   1056.5409   1071.4588   1075.4406   1308.0317
   1391.8988   1399.9264   1404.4085   1414.5751   1464.2157   1476.7322   1481.4100
   1496.8874   1557.9665   2994.4002   3004.3717   3036.3261   3044.5403   3115.2055
   3120.4182   3147.0915   3234.8475   3703.7634

== Thermochemistry energies (hartree) ==
  ZPVE =     0.121557  (after scaling by 0.9854)
G4  Ee =  -308.049384  (total electronic energy)
G4  U0 =  -307.927827  (Zero-kelvin internal energy)
G4  UT =  -307.919340  (Internal energy at 298.15 K)
G4  HT =  -307.918396  (Enthalpy at 298.15 K)
G4  GT =  -307.961625  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.369856   -0.045266    0.889691
H     0.615820    0.840185    1.489502
H     0.567986   -0.961232    1.460835
C    -0.927765    0.003336    0.179553
H     2.802991    0.684055   -0.785927
C    -1.546771    1.315957   -0.161044
H    -1.890487    1.345794   -1.201454
H    -2.435614    1.489760    0.465818
H    -0.854061    2.143589    0.004235
C    -1.605870   -1.261315   -0.223851
H    -1.972642   -1.215272   -1.255554
H    -0.940613   -2.121240   -0.125659
H    -2.486409   -1.439124    0.413770
O     0.935896   -0.041339   -0.384809
O     2.671145   -0.064009   -0.186649

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -683.5304     80.1715    102.6319    117.5234    148.6187    190.7589    205.2384
    283.8381    383.3714    400.3470    430.8313    764.9930    923.3340    944.9503
    975.6729    995.7349   1016.3299   1050.9799   1108.1678   1177.5046   1283.6137
   1312.6355   1366.1317   1400.4501   1408.4072   1458.9490   1473.5422   1476.8282
   1497.6605   1535.5182   2987.6079   2992.6064   3003.9902   3053.5986   3058.1142
   3061.6626   3127.8008   3131.5063   3784.5739

== Thermochemistry energies (hartree) ==
  ZPVE =     0.120588  (after scaling by 0.9854)
G4  Ee =  -308.053652  (total electronic energy)
G4  U0 =  -307.933064  (Zero-kelvin internal energy)
G4  UT =  -307.924386  (Internal energy at 298.15 K)
G4  HT =  -307.923442  (Enthalpy at 298.15 K)
G4  GT =  -307.966710  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 4: tertbutyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.264664    0.783864    0.013355
C     0.000008   -0.000005   -0.134946
C     0.046515   -1.487151    0.013542
C    -1.311181    0.703292    0.013307
H     1.182679    1.777723   -0.441884
H     2.118254    0.268315   -0.441971
H     1.532720    0.949937    1.073161
H    -0.826852   -1.968649   -0.441553
H     0.056521   -1.802185    1.073391
H     0.948116   -1.913172   -0.441812
H    -1.291483    1.700313   -0.441980
H    -1.589123    0.852341    1.073101
H    -2.130871    0.135376   -0.442000

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    123.2728    123.6089    131.2708    252.2070    376.4529    376.6554    757.2497
    938.6131    938.7280    969.4987   1008.9608   1008.9803   1092.0314   1295.4554
   1295.5099   1395.6215   1395.7256   1425.7090   1469.1104   1469.2087   1469.4898
   1486.6754   1493.5898   1493.6417   2931.9480   2931.9841   2941.2324   3036.1472
   3036.2000   3039.1111   3081.3068   3086.1657   3086.2203

== Thermochemistry energies (hartree) ==
  ZPVE =     0.114395  (after scaling by 0.9854)
G4  Ee =  -157.760072  (total electronic energy)
G4  U0 =  -157.645677  (Zero-kelvin internal energy)
G4  UT =  -157.639188  (Internal energy at 298.15 K)
G4  HT =  -157.638243  (Enthalpy at 298.15 K)
G4  GT =  -157.675341  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.670221    0.665848    1.268616
C     0.115893    0.347516    0.000000
C     1.507894    0.970390    0.000000
C    -0.670221    0.665848   -1.268616
H    -0.902855    1.734023    1.306737
H    -0.091129    0.406699    2.159548
H    -1.605285    0.102352    1.282588
H     1.428151    2.060982    0.000000
H     2.070016    0.666564   -0.887370
H     2.070016    0.666564    0.887370
O     0.411507   -1.116860    0.000000
H    -0.091129    0.406699   -2.159548
H    -0.902855    1.734023   -1.306737
H    -1.605285    0.102352   -1.282588
O    -0.670221   -1.855374   -0.000000

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    126.0559    172.5711    224.9672    239.4009    269.9578    328.9661    359.6683
    399.2484    435.6013    545.1539    736.3890    807.3895    927.7066    929.5238
    965.2009   1037.6505   1052.2053   1181.0712   1233.3776   1260.8641   1293.3529
   1392.9396   1397.1767   1422.5851   1466.9053   1485.0800   1486.3781   1494.4812
   1495.5415   1519.1530   3044.5444   3045.4914   3051.6080   3115.9037   3118.0949
   3123.0115   3125.2736   3136.1547   3140.0017

== Thermochemistry energies (hartree) ==
  ZPVE =     0.124787  (after scaling by 0.9854)
G4  Ee =  -308.108400  (total electronic energy)
G4  U0 =  -307.983613  (Zero-kelvin internal energy)
G4  UT =  -307.975927  (Internal energy at 298.15 K)
G4  HT =  -307.974983  (Enthalpy at 298.15 K)
G4  GT =  -308.015061  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.276401   -0.426436    1.502048
C     0.391802    0.015927    0.078813
C     1.607920   -0.625882   -0.607347
C     0.409310    1.539954   -0.052448
H     0.107082    0.277965    2.307478
H     0.323437   -1.484076    1.740628
H     2.530695   -0.262822   -0.147709
H     1.617940   -0.368749   -1.670480
H     1.575652   -1.714611   -0.513060
O    -0.703551   -0.541327   -0.706093
H     0.492249    1.828656   -1.103640
H     1.259439    1.959652    0.494440
H    -0.511473    1.965007    0.351621
O    -1.958037   -0.022160   -0.218092
H    -2.214917   -0.714507    0.407806

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    113.3800    144.3911    199.8228    235.6051    250.7806    270.8795    324.0567
    350.5107    396.4592    448.6538    493.4824    584.9413    767.5594    838.7171
    912.2380    941.2065    951.7301    981.1233   1033.3315   1156.2567   1261.3016
   1272.4299   1385.7908   1388.7479   1404.9468   1456.0994   1473.5486   1484.6383
   1489.9310   1509.3573   3042.7800   3047.3290   3115.9492   3121.4435   3127.1629
   3137.6074   3143.4885   3254.9628   3741.9395

== Thermochemistry energies (hartree) ==
  ZPVE =     0.121796  (after scaling by 0.9854)
G4  Ee =  -308.077032  (total electronic energy)
G4  U0 =  -307.955236  (Zero-kelvin internal energy)
G4  UT =  -307.946751  (Internal energy at 298.15 K)
G4  HT =  -307.945807  (Enthalpy at 298.15 K)
G4  GT =  -307.987380  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.052805    0.932113    1.283142
C    -0.052805    0.130594    0.000000
C    -0.576412   -1.243896   -0.000000
C    -0.052805    0.932113   -1.283142
H    -0.017656    0.271445    2.152650
H    -0.950137    1.556461    1.353379
H     0.818908    1.594574    1.321459
H    -0.950137    1.556461   -1.353379
H    -0.017656    0.271445   -2.152650
H     0.818908    1.594574   -1.321459
O     0.832730   -1.000942   -0.000000
H    -0.977554   -1.671483   -0.918593
H    -0.977554   -1.671483    0.918593

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    179.6030    217.1014    350.5030    358.3323    406.1078    408.5472    704.3365
    819.1405    904.8970    931.7381    955.3221   1017.9411   1076.7892   1134.1790
   1149.2917   1173.5645   1282.5037   1394.2902   1409.6260   1421.4209   1473.7738
   1485.9881   1493.5316   1505.9467   1536.4685   3031.3025   3036.3834   3074.7740
   3093.4869   3098.3991   3122.4915   3124.6722   3158.3729

== Thermochemistry energies (hartree) ==
  ZPVE =     0.111192  (after scaling by 0.9854)
G4  Ee =  -232.384120  (total electronic energy)
G4  U0 =  -232.272928  (Zero-kelvin internal energy)
G4  UT =  -232.267081  (Internal energy at 298.15 K)
G4  HT =  -232.266137  (Enthalpy at 298.15 K)
G4  GT =  -232.301294  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.274947   -0.677941    0.000003
C     0.000000    0.124566   -0.000002
C     0.000001    1.456978   -0.000016
C    -1.274949   -0.677939    0.000011
H     2.159636   -0.036470   -0.000009
H     1.327183   -1.334165   -0.878355
H     1.327191   -1.334143    0.878378
H    -1.327192   -1.334163   -0.878347
H    -2.159636   -0.036467    0.000006
H    -1.327187   -1.334141    0.878386
H     0.923232    2.027782   -0.000025
H    -0.923229    2.027784   -0.000019

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    176.6651    213.5577    376.2478    435.0083    442.6857    708.8943    817.1783
    927.1980    962.8198    987.0313   1023.8777   1087.9719   1107.6406   1295.7868
   1407.9467   1413.5192   1448.0732   1470.7393   1483.9391   1488.7150   1503.0376
   1729.3903   3013.1169   3018.9421   3059.9435   3063.1561   3114.0538   3116.0626
   3141.8320   3220.9491

== Thermochemistry energies (hartree) ==
  ZPVE =     0.106085  (after scaling by 0.9854)
G4  Ee =  -157.194053  (total electronic energy)
G4  U0 =  -157.087968  (Zero-kelvin internal energy)
G4  UT =  -157.082615  (Internal energy at 298.15 K)
G4  HT =  -157.081671  (Enthalpy at 298.15 K)
G4  GT =  -157.115288  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.372826    0.008355    0.040585
C    -0.236138   -0.498096    1.359266
H    -1.476209   -0.258619    0.796129
H    -0.201663   -1.575562    1.522698
H    -0.084873    0.095961    2.258381
C     0.560740    1.527501    0.063677
H     1.286323    1.819802    0.829186
H     0.923609    1.875630   -0.907287
H    -0.391069    2.019755    0.275106
C     1.640321   -0.733387   -0.372403
H     1.458265   -1.809841   -0.421065
H     1.979433   -0.392295   -1.355563
H     2.441370   -0.543791    0.348132
O    -0.637794   -0.364423   -0.931450
O    -1.857417   -0.017738   -0.305109

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2231.4979    184.3805    195.8098    235.3007    296.4683    334.5726    384.9046
    402.6659    507.6488    567.2536    644.0959    785.5188    842.3258    907.8318
    927.1174    954.2801    966.8381   1012.6681   1040.7548   1100.7052   1173.6767
   1248.3147   1271.0324   1393.6387   1409.1623   1450.9344   1475.5336   1484.3728
   1492.5849   1506.7166   1731.8015   3040.5773   3045.7138   3100.1902   3111.6740
   3117.3681   3126.1038   3134.0792   3194.9446

== Thermochemistry energies (hartree) ==
  ZPVE =     0.118530  (after scaling by 0.9854)
G4  Ee =  -308.043652  (total electronic energy)
G4  U0 =  -307.925122  (Zero-kelvin internal energy)
G4  UT =  -307.918063  (Internal energy at 298.15 K)
G4  HT =  -307.917119  (Enthalpy at 298.15 K)
G4  GT =  -307.955747  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.715738    0.000002    0.230851
C     0.069054    0.000018    1.463942
H    -1.197520    0.000015    0.960216
H     0.072095   -0.917957    2.049643
H     0.072099    0.918005    2.049622
C     1.206808    1.277295   -0.386596
H     2.279120    1.397157   -0.175674
H     1.088158    1.270558   -1.473463
H     0.687984    2.148859    0.019137
C     1.206805   -1.277306   -0.386567
H     0.687975   -2.148858    0.019183
H     1.088161   -1.270591   -1.473434
H     2.279115   -1.397168   -0.175636
O    -1.236465   -0.000011   -0.951247
O    -2.044486    0.000002    0.035076

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1047.5928    129.7085    164.8438    197.7137    202.5941    207.6974    366.2211
    429.1272    444.3645    533.0643    624.9948    654.8688    817.8421    940.2220
    984.3036   1022.4952   1025.0516   1071.6675   1100.2730   1274.7115   1321.2753
   1339.9119   1405.7946   1408.9184   1427.8819   1467.4822   1476.6219   1482.9129
   1496.5529   1578.5098   1619.1443   3011.5623   3016.5243   3085.7825   3088.7064
   3101.4694   3127.4398   3129.9137   3182.1822

== Thermochemistry energies (hartree) ==
  ZPVE =     0.118891  (after scaling by 0.9854)
G4  Ee =  -308.053530  (total electronic energy)
G4  U0 =  -307.934639  (Zero-kelvin internal energy)
G4  UT =  -307.927030  (Internal energy at 298.15 K)
G4  HT =  -307.926086  (Enthalpy at 298.15 K)
G4  GT =  -307.966355  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.655391    0.114998    0.153529
C     0.651841   -0.150869    1.517171
H    -2.199375    0.541696   -0.669405
H     1.051171   -1.081014    1.904207
H     0.132576    0.496999    2.214054
C     0.333834    1.511421   -0.322948
H     1.215659    2.156294   -0.232603
H     0.037124    1.507776   -1.376560
H    -0.466639    1.957540    0.273168
C     1.557486   -0.695185   -0.747638
H     1.685129   -1.711784   -0.368296
H     1.142390   -0.751950   -1.757133
H     2.547004   -0.227580   -0.812365
O    -0.939829   -0.805023   -0.360064
O    -2.102215   -0.141249    0.013095

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -499.2560     91.7817    148.6988    188.8117    198.3513    239.8039    314.9821
    382.0992    391.3239    443.0534    451.0363    520.8982    787.4810    795.4557
    944.1816    957.3720    970.4672   1017.6732   1060.7209   1076.0022   1300.4432
   1378.8552   1398.4841   1408.6609   1416.6923   1474.0676   1485.0029   1486.2539
   1506.0389   1527.2856   3030.7054   3036.5057   3090.9752   3102.7552   3117.9343
   3129.2631   3153.8546   3249.4264   3686.5222

== Thermochemistry energies (hartree) ==
  ZPVE =     0.121135  (after scaling by 0.9854)
G4  Ee =  -308.048454  (total electronic energy)
G4  U0 =  -307.927319  (Zero-kelvin internal energy)
G4  UT =  -307.919131  (Internal energy at 298.15 K)
G4  HT =  -307.918186  (Enthalpy at 298.15 K)
G4  GT =  -307.959591  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.485965    0.045591    0.032172
C     1.266556   -1.198657   -0.179346
H    -2.450303   -0.532641    0.482831
H     1.591359   -1.479354   -1.172988
H     1.407715   -1.898260    0.634468
C     0.433215    0.550378    1.469510
H     1.351356    1.084647    1.732291
H    -0.415487    1.229279    1.578821
H     0.300981   -0.283015    2.165628
C     0.703056    1.154051   -0.990371
H     0.724776    0.740947   -2.002170
H    -0.120453    1.869982   -0.930370
H     1.642704    1.683020   -0.801943
O    -0.598535   -0.797886   -0.298478
O    -2.072139    0.082538   -0.161317

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -747.0767    112.2816    183.9330    198.5332    211.2047    241.9407    332.8771
    347.3695    399.4794    407.4408    477.4378    534.1167    743.0905    759.8824
    878.3086    909.0007    952.2113    987.2751   1025.8250   1038.6092   1159.9725
   1264.9142   1330.8419   1395.1037   1407.1728   1461.8071   1470.9165   1487.3514
   1496.2527   1508.7835   3040.5299   3045.8839   3113.1257   3118.4283   3129.4457
   3133.9574   3165.9413   3284.8293   3785.0211

== Thermochemistry energies (hartree) ==
  ZPVE =     0.120195  (after scaling by 0.9854)
G4  Ee =  -308.054482  (total electronic energy)
G4  U0 =  -307.934287  (Zero-kelvin internal energy)
G4  UT =  -307.926141  (Internal energy at 298.15 K)
G4  HT =  -307.925197  (Enthalpy at 298.15 K)
G4  GT =  -307.966177  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 5: neopentyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.000001    1.327303   -0.747447
C     0.000000   -0.001428    0.054926
C     1.260900   -0.808472   -0.314136
C    -1.260899   -0.808474   -0.314136
C    -0.000000    0.303555    1.523194
H     0.885036    1.927597   -0.514074
H    -0.885039    1.927596   -0.514074
H    -0.000001    1.126867   -1.825838
H     0.928479    0.509853    2.045474
H    -0.928479    0.509853    2.045474
H    -2.170734   -0.254196   -0.059226
H    -1.287893   -1.762520    0.221893
H    -1.289093   -1.021621   -1.388353
H     2.170734   -0.254192   -0.059227
H     1.289094   -1.021619   -1.388353
H     1.287896   -1.762518    0.221893

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    108.8434    214.9250    267.1957    273.5449    304.0713    326.6916    382.7231
    410.3325    412.2809    534.1308    739.0901    908.3338    914.5118    948.0851
    949.5275    956.9399   1030.8638   1076.2013   1202.0073   1265.8686   1277.4661
   1388.8223   1395.4537   1417.5476   1463.5088   1476.6626   1483.5356   1485.4398
   1500.6950   1501.8751   1517.3833   3018.6206   3023.2768   3029.3599   3087.5817
   3091.6276   3096.4831   3097.9181   3102.6619   3104.3333   3136.0195   3239.9475


== Thermochemistry energies (hartree) ==
  ZPVE =     0.141794  (after scaling by 0.9854)
G4  Ee =  -197.062310  (total electronic energy)
G4  U0 =  -196.920516  (Zero-kelvin internal energy)
G4  UT =  -196.913009  (Internal energy at 298.15 K)
G4  HT =  -196.912065  (Enthalpy at 298.15 K)
G4  GT =  -196.950975  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.031340   -0.954656    1.158476
C     0.740929    0.031559    0.012901
C     1.943159    0.086254   -0.948526
C     0.463499    1.434591    0.579359
C    -0.460430   -0.464470   -0.809507
H     1.255373   -1.956030    0.774073
H     0.177052   -1.036749    1.835999
H     1.895326   -0.619728    1.741314
H    -0.721579    0.227160   -1.613862
H    -0.266128   -1.462048   -1.217512
H    -0.399436    1.434272    1.250049
H     0.262776    2.154425   -0.220804
H     1.331651    1.790596    1.144017
H     2.166081   -0.899971   -1.370538
H     2.836764    0.430900   -0.418552
H     1.761646    0.777242   -1.778999
O    -1.653556   -0.636250    0.004260
O    -2.422758    0.431283   -0.014435

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     71.0672    105.9698    208.5114    230.3362    259.0705    265.3123    305.0684
    334.7490    388.1753    403.4789    473.9095    560.7057    741.0184    887.2920
    917.9428    936.2692    945.2184    962.1148    964.7476   1047.4077   1085.2796
   1175.3989   1233.4666   1251.7446   1275.7094   1319.2327   1367.7606   1400.1459
   1403.4345   1434.2694   1464.7903   1478.7436   1484.0297   1487.1887   1505.6944
   1506.0226   1518.3309   3025.4825   3030.6918   3036.5259   3050.6099   3093.1071
   3096.9592   3098.7771   3103.8421   3115.1956   3120.1131   3121.5613

== Thermochemistry energies (hartree) ==
  ZPVE =     0.153310  (after scaling by 0.9854)
G4  Ee =  -347.407740  (total electronic energy)
G4  U0 =  -347.254430  (Zero-kelvin internal energy)
G4  UT =  -347.245569  (Internal energy at 298.15 K)
G4  HT =  -347.244625  (Enthalpy at 298.15 K)
G4  GT =  -347.287973  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.058956   -0.795635    1.261815
C     0.750427    0.070645    0.027621
C     1.989039    0.117309   -0.907068
C     0.389655    1.466929    0.439461
C    -0.399121   -0.580378   -0.786791
H     1.388161   -1.796984    0.964601
H     0.170998   -0.907675    1.889365
H     1.854964   -0.345675    1.863834
H    -0.618907   -0.000107   -1.691078
H    -0.104071   -1.595535   -1.081678
H    -1.828761    0.959240    0.675492
H     0.075829    2.188022   -0.309390
H     0.687815    1.850989    1.409651
H     2.261905   -0.891576   -1.238529
H     2.849418    0.546707   -0.385928
H     1.794204    0.727021   -1.795212
O    -1.594058   -0.774146   -0.048382
O    -2.314103    0.473191   -0.015537

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     87.2033    165.1329    179.9923    217.8994    242.9359    258.0843    290.5005
    336.8659    358.8319    394.8861    398.5728    456.1117    557.6268    627.7745
    759.4759    876.2293    898.9845    931.1946    950.3799    953.3950   1013.4022
   1027.7867   1064.3348   1166.8421   1242.7676   1254.4294   1325.2228   1371.1990
   1391.6466   1413.0373   1422.6122   1449.7288   1466.0289   1483.4954   1489.0000
   1501.2830   1508.6335   3017.6678   3024.7557   3035.0804   3073.2178   3093.7165
   3100.4292   3110.1718   3119.1926   3132.3407   3236.7064   3620.5148

== Thermochemistry energies (hartree) ==
  ZPVE =     0.150627  (after scaling by 0.9854)
G4  Ee =  -347.377975  (total electronic energy)
G4  U0 =  -347.227348  (Zero-kelvin internal energy)
G4  UT =  -347.218009  (Internal energy at 298.15 K)
G4  HT =  -347.217065  (Enthalpy at 298.15 K)
G4  GT =  -347.260839  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.260971    1.234725    0.000000
C    -0.018871    0.401496    0.000000
C    -1.266125    1.280025    0.000000
C    -0.018871   -0.755505    1.035261
C    -0.018871   -0.755505   -1.035261
H     1.310190    1.879850   -0.884691
H     2.149910    0.595683    0.000000
H     1.310190    1.879850    0.884691
H    -0.941948   -0.854767   -1.622703
H     0.840768   -0.790918   -1.716928
H    -1.291317    1.927512   -0.884033
H    -1.291317    1.927512    0.884033
H    -2.179524    0.676493    0.000000
O     0.070603   -1.753368    0.000000
H    -0.941948   -0.854767    1.622703
H     0.840768   -0.790918    1.716928

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     28.6333    219.3045    256.1844    311.0449    338.3020    387.5222    404.7938
    639.5212    854.4911    884.4220    927.6825    937.9738    963.4545    973.1452
   1026.3975   1042.2966   1062.6307   1157.5666   1162.2205   1219.8074   1267.1305
   1294.0793   1311.5138   1381.8290   1404.2603   1425.8525   1485.3019   1487.9024
   1501.5666   1503.5411   1517.7734   1538.1478   2992.3117   3003.0006   3020.5041
   3026.7430   3040.9596   3042.5344   3085.9390   3090.9349   3097.3005   3099.4677


== Thermochemistry energies (hartree) ==
  ZPVE =     0.140118  (after scaling by 0.9854)
G4  Ee =  -271.686562  (total electronic energy)
G4  U0 =  -271.546444  (Zero-kelvin internal energy)
G4  UT =  -271.539570  (Internal energy at 298.15 K)
G4  HT =  -271.538626  (Enthalpy at 298.15 K)
G4  GT =  -271.577463  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.325409    0.915297    1.275407
C    -0.050548    0.142166    0.000000
C    -0.325409    0.915297   -1.275407
C    -0.325409   -1.342603   -0.000000
C     1.099908   -0.835867   -0.000000
H     0.291689    1.820219    1.330407
H    -0.110892    0.311918    2.163089
H    -1.375252    1.227584    1.330414
H     0.291689    1.820219   -1.330407
H    -1.375252    1.227584   -1.330414
H    -0.110892    0.311918   -2.163089
H     1.680279   -0.947242    0.910105
H     1.680279   -0.947242   -0.910105
H    -0.705220   -1.795349   -0.910105
H    -0.705220   -1.795349    0.910105

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    215.9368    241.7437    325.9036    348.4854    357.0697    393.0891    688.9301
    786.0570    853.8812    896.0332    949.2381    951.2559    974.3221   1047.4254
   1066.9667   1077.4372   1093.2575   1158.7847   1187.9761   1319.4493   1353.2494
   1411.7120   1425.2540   1468.5277   1481.3189   1493.8431   1500.4731   1501.8576
   1517.4532   3016.0462   3020.9301   3074.9091   3078.0182   3095.2401   3097.6902
   3123.3827   3128.4574   3200.5679   3215.2747

== Thermochemistry energies (hartree) ==
  ZPVE =     0.135003  (after scaling by 0.9854)
G4  Ee =  -196.490148  (total electronic energy)
G4  U0 =  -196.355145  (Zero-kelvin internal energy)
G4  UT =  -196.349127  (Internal energy at 298.15 K)
G4  HT =  -196.348183  (Enthalpy at 298.15 K)
G4  GT =  -196.383513  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.707621    0.050795    0.025585
C     0.155263    1.381000    0.498056
H     0.358657    1.668153    1.528742
H     0.208694    2.209586   -0.209104
H    -1.223708    1.089792    0.445048
C     1.053353   -0.845661    1.227089
H     0.164997   -1.039709    1.833694
H     1.453621   -1.809738    0.895174
H     1.807755   -0.369639    1.861566
C     1.946795    0.256023   -0.872942
H     2.319164   -0.704687   -1.246667
H     1.713831    0.889239   -1.735130
H     2.755409    0.734304   -0.312339
C    -0.388279   -0.653030   -0.835716
H    -0.577274   -0.091908   -1.759244
H    -0.089781   -1.678456   -1.078457
O    -2.131098    0.519684    0.034157
O    -1.586388   -0.773646   -0.093621

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1605.6490    108.1243    224.5915    244.1848    273.4482    304.0114    322.7042
    387.6454    427.3557    451.9003    484.9495    543.5839    645.4734    760.9019
    882.1819    919.7971    939.4532    946.1228    968.3819    999.0851   1029.0634
   1049.6840   1070.6299   1121.3092   1202.3877   1225.8430   1245.8331   1310.6409
   1358.8456   1395.0754   1414.9614   1455.5571   1466.1439   1485.4191   1491.9985
   1502.2175   1508.6928   1590.9000   3021.6921   3027.2940   3034.8578   3089.1816
   3091.2640   3095.5801   3100.8652   3108.2014   3121.1036   3180.4491

== Thermochemistry energies (hartree) ==
  ZPVE =     0.147332  (after scaling by 0.9854)
G4  Ee =  -347.361867  (total electronic energy)
G4  U0 =  -347.214535  (Zero-kelvin internal energy)
G4  UT =  -347.206575  (Internal energy at 298.15 K)
G4  HT =  -347.205631  (Enthalpy at 298.15 K)
G4  GT =  -347.246559  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.031913   -0.000044   -0.941171
H     0.418042    0.920243   -1.354649
H     0.418031   -0.920370   -1.354573
C    -1.120674   -0.000001   -0.041159
C    -0.004454    0.000019    1.036315
H    -0.046919   -0.910747    1.637091
H     1.209505    0.000044    0.800401
H    -0.046941    0.910793    1.637079
C    -1.967402   -1.269469   -0.051895
H    -2.613986   -1.309104    0.831076
H    -2.606181   -1.304493   -0.941146
H    -1.340051   -2.166300   -0.051616
O     2.607255    0.000043    0.589778
O     2.559806   -0.000045   -0.682576
C    -1.967366    1.269491   -0.051973
H    -2.606153    1.304472   -0.941220
H    -2.613940    1.309203    0.831002
H    -1.339990    2.166304   -0.051762

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1197.7290     47.6764     88.8905    161.5293    225.5008    239.4134    296.1958
    325.1977    347.0991    402.1830    425.7155    457.9610    467.5945    717.3041
    756.3570    840.8098    867.8665    926.3670    950.3572    955.4542    979.4916
   1006.4199   1044.9811   1068.7682   1189.1560   1266.6604   1331.1664   1344.6917
   1400.7154   1418.7140   1419.7343   1425.3798   1474.1593   1484.0381   1489.8701
   1503.8453   1511.3359   1697.1889   3027.1118   3031.5950   3051.1331   3096.4920
   3100.9060   3103.6402   3106.3536   3150.4408   3196.6449   3305.1083

== Thermochemistry energies (hartree) ==
  ZPVE =     0.145302  (after scaling by 0.9854)
G4  Ee =  -347.292646  (total electronic energy)
G4  U0 =  -347.147344  (Zero-kelvin internal energy)
G4  UT =  -347.138193  (Internal energy at 298.15 K)
G4  HT =  -347.137248  (Enthalpy at 298.15 K)
G4  GT =  -347.181759  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.049011    0.043601    0.025651
C    -0.165364   -0.227727    1.186515
H    -0.052370   -1.231720    1.571359
H     0.461435    0.551108    1.597018
H     3.001752    0.679735   -0.779598
C    -1.509689    1.496357   -0.088671
H    -0.668254    2.185775    0.031322
H    -1.966629    1.683744   -1.066613
H    -2.249494    1.728664    0.684675
C    -2.199168   -0.949252   -0.138701
H    -2.681058   -0.830474   -1.115199
H    -1.843969   -1.981645   -0.059463
H    -2.955810   -0.793124    0.637823
C     0.173274   -0.280069   -0.789057
H     0.174512   -1.239297   -1.294003
H     0.614926    0.545834   -1.335153
O     2.653934    0.481247    0.102985
O     1.929154   -0.705755   -0.108809

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -706.3751     53.2946     67.3227    223.1554    225.6268    242.4401    286.2744
    331.6585    347.5225    380.3616    398.9499    414.2176    452.1004    581.1468
    684.6869    743.5738    851.7382    903.6147    923.0232    945.6122    959.9244
   1028.6694   1035.2920   1074.7812   1098.1586   1193.1657   1298.8853   1310.5084
   1379.7566   1400.5499   1411.8510   1426.3033   1471.6460   1484.1403   1486.8906
   1501.5590   1507.2382   3025.1643   3029.8026   3095.3140   3099.5748   3101.5003
   3105.4016   3124.9203   3179.9183   3235.8153   3293.2930   3701.1615

== Thermochemistry energies (hartree) ==
  ZPVE =     0.148428  (after scaling by 0.9854)
G4  Ee =  -347.294700  (total electronic energy)
G4  U0 =  -347.146272  (Zero-kelvin internal energy)
G4  UT =  -347.136934  (Internal energy at 298.15 K)
G4  HT =  -347.135990  (Enthalpy at 298.15 K)
G4  GT =  -347.180652  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.905787   -0.005947   -0.008853
C     0.391071   -0.276269    1.390187
H     0.309437   -1.300194    1.739532
H     0.404407    0.496215    2.150188
H    -3.226307   -0.595091    0.187906
C     2.003511   -0.981204   -0.452335
H     1.685113   -2.021438   -0.329320
H     2.253873   -0.828862   -1.508184
H     2.917413   -0.834726    0.133115
C     1.366448    1.451386   -0.144679
H     1.659802    1.672227   -1.176148
H     0.559454    2.135418    0.134657
H     2.227209    1.653121    0.502060
C    -0.438902   -0.224744   -0.730181
H    -0.663275    0.499304   -1.519671
H    -0.548413   -1.240062   -1.134908
O    -2.811338    0.104768   -0.334660
O    -1.306938   -0.031674    0.396651

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -797.1603     69.5151    155.1632    161.2733    212.0226    238.1732    280.8123
    312.9241    325.1845    397.4341    409.7355    427.1864    541.7103    569.9247
    782.0455    824.4674    908.3469    927.0065    953.0595    965.8197   1000.7186
   1018.3693   1057.6717   1098.0342   1186.8083   1224.9432   1243.5286   1285.1634
   1345.3556   1397.7914   1414.7608   1466.6020   1486.0585   1487.0909   1500.8982
   1509.9006   1521.1248   3005.8321   3025.3408   3031.3651   3075.1656   3094.2501
   3099.7287   3101.2192   3110.8377   3142.8649   3249.2998   3789.3543

== Thermochemistry energies (hartree) ==
  ZPVE =     0.149133  (after scaling by 0.9854)
G4  Ee =  -347.344800  (total electronic energy)
G4  U0 =  -347.195667  (Zero-kelvin internal energy)
G4  UT =  -347.186551  (Internal energy at 298.15 K)
G4  HT =  -347.185607  (Enthalpy at 298.15 K)
G4  GT =  -347.229320  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 6:cyclohexyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.289714    0.777406    0.154692
C    -0.000000    1.463349   -0.164195
C     1.289714    0.777406    0.154691
C     1.266342   -0.712975   -0.243361
C     0.000000   -1.409192    0.273809
C    -1.266342   -0.712975   -0.243360
H    -2.163581   -1.215348    0.135350
H    -1.296382   -0.791972   -1.337963
H     0.000000   -1.396410    1.373338
H     0.000000   -2.463805   -0.024652
H     2.163581   -1.215348    0.135349
H     1.296381   -0.791972   -1.337964
H     1.485957    0.835247    1.243224
H     2.132813    1.289252   -0.323031
H    -0.000000    2.527742   -0.377500
H    -2.132813    1.289252   -0.323030
H    -1.485956    0.835247    1.243225

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    171.5231    206.4998    327.7852    388.1792    433.8644    455.9492    606.4854
    779.0405    808.7995    851.5860    873.8909    876.2477    923.2190   1015.0144
   1033.3325   1057.7189   1090.2710   1110.2676   1128.5356   1150.6358   1252.4261
   1281.0151   1291.6657   1338.6534   1344.8544   1354.0171   1378.5517   1389.3111
   1393.8900   1464.4832   1468.8779   1485.4495   1488.3374   1500.6566   2903.6520
   2908.8652   3004.9342   3018.1370   3019.0742   3051.2830   3051.8901   3058.6398
   3062.1411   3066.9810   3170.7073

== Thermochemistry energies (hartree) ==
  ZPVE =     0.152737  (after scaling by 0.9854)
G4  Ee =  -235.164307  (total electronic energy)
G4  U0 =  -235.011570  (Zero-kelvin internal energy)
G4  UT =  -235.005405  (Internal energy at 298.15 K)
G4  HT =  -235.004461  (Enthalpy at 298.15 K)
G4  GT =  -235.041393  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.130395    1.153038   -0.275173
C    -0.648726   -0.188011    0.236961
C     0.237173   -1.354433   -0.184449
C     1.683088   -1.122138    0.284905
C     2.229623    0.224816   -0.210738
C     1.311921    1.385733    0.200442
H     1.685777    2.332501   -0.203040
H     1.322967    1.488545    1.294130
H     2.313541    0.200565   -1.305775
H     3.241494    0.386025    0.176383
H     2.317838   -1.944806   -0.060218
H     1.715229   -1.145012    1.382700
H     0.209078   -1.438383   -1.278383
H    -0.160180   -2.290844    0.219915
H    -0.772750   -0.159330    1.325095
O    -1.981234   -0.452330   -0.311363
O    -2.894504    0.312873    0.241911
H    -0.798125    1.949383    0.065459
H    -0.165065    1.143000   -1.372339

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     80.7701    130.9883    223.3433    248.8593    321.3116    364.8351    438.5234
    453.7305    505.0543    565.5788    796.4357    807.1287    848.6957    895.1154
    902.9297    923.3738    936.5556   1021.0678   1046.5752   1062.7796   1085.3921
   1103.5047   1171.7975   1200.0577   1217.8973   1269.0096   1281.3432   1285.2168
   1327.1885   1331.5568   1365.5534   1376.3046   1378.0483   1382.2905   1392.3982
   1484.2524   1486.6988   1489.7141   1494.9060   1509.3067   3013.7951   3016.5105
   3021.6774   3028.7015   3031.2122   3054.0778   3068.9770   3071.1843   3074.9894
   3084.2876   3095.7828

== Thermochemistry energies (hartree) ==
  ZPVE =     0.163356  (after scaling by 0.9854)
G4  Ee =  -385.512275  (total electronic energy)
G4  U0 =  -385.348919  (Zero-kelvin internal energy)
G4  UT =  -385.341113  (Internal energy at 298.15 K)
G4  HT =  -385.340169  (Enthalpy at 298.15 K)
G4  GT =  -385.381858  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.630199   -0.211836    0.248051
C     0.313718   -1.354822   -0.159007
C     1.749632   -1.064434    0.301947
C     2.265993    0.262949   -0.268201
C     1.342449    1.434527    0.125148
C    -0.092586    1.122644   -0.150119
H    -0.799995    1.904923   -0.397283
H     1.642853    2.353375   -0.389769
H     1.488226    1.637649    1.203542
H     2.309372    0.191697   -1.362313
H     3.286533    0.456830    0.079826
H     2.404131   -1.889007   -0.000691
H     1.782175   -1.029085    1.400015
H     0.284659   -1.446989   -1.251248
H    -0.052790   -2.297954    0.258356
O    -1.881289   -0.520054   -0.370825
O    -2.858028    0.437834    0.095357
H    -3.350193   -0.103416    0.729377
H    -0.774478   -0.254438    1.347002

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     94.8538    117.1044    184.7921    215.5772    240.4024    313.8362    347.0143
    371.8135    452.2197    490.7825    528.9217    602.6175    793.1464    838.2094
    868.0820    904.0681    909.5558    946.8242    969.0318   1038.0551   1059.9902
   1069.0537   1102.4693   1109.2457   1148.9798   1202.4084   1255.6556   1274.8375
   1311.7425   1323.4937   1346.0670   1351.2462   1367.7587   1380.6333   1384.4985
   1396.4366   1469.1458   1486.4575   1489.9257   1500.6822   2876.4886   2913.4322
   3011.1879   3024.9376   3036.6561   3060.0471   3066.0736   3071.1654   3085.3667
   3205.8644   3744.2720

== Thermochemistry energies (hartree) ==
  ZPVE =     0.160181  (after scaling by 0.9854)
G4  Ee =  -385.485087  (total electronic energy)
G4  U0 =  -385.324906  (Zero-kelvin internal energy)
G4  UT =  -385.316250  (Internal energy at 298.15 K)
G4  HT =  -385.315306  (Enthalpy at 298.15 K)
G4  GT =  -385.358502  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.987973    0.836146   -0.293602
C     0.345659    1.517624   -0.036399
C     1.551305    0.569982   -0.171247
C     1.275483   -0.808440    0.442380
C     0.125878   -1.510810   -0.295164
C    -1.097820   -0.629178   -0.411192
H    -1.922940   -1.040301   -0.995762
O    -1.509372    0.041046    0.783254
H    -0.147114   -2.444870    0.210846
H     0.443762   -1.786539   -1.310268
H     1.012041   -0.697397    1.500002
H     2.174509   -1.431806    0.397814
H     2.432485    1.028225    0.290120
H     1.791086    0.439293   -1.235226
H     0.309661    1.943617    0.973939
H     0.455301    2.362623   -0.725348
H    -1.749011    1.446837   -0.780806

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    142.7122    270.4089    355.0371    371.2494    438.4170    540.7891    644.7581
    774.3019    786.4238    826.4033    850.9347    894.3645    905.3565    986.5031
   1002.9939   1043.9634   1053.2786   1078.5679   1099.4618   1169.5073   1191.4942
   1211.3659   1274.7573   1290.6997   1302.6803   1352.7872   1369.7690   1377.2718
   1389.2011   1398.2659   1462.4341   1477.6210   1485.2093   1488.6819   1499.2601
   3013.9252   3015.5638   3028.6092   3039.4644   3055.3020   3064.0549   3073.2630
   3085.5623   3087.0391   3103.0084

== Thermochemistry energies (hartree) ==
  ZPVE =     0.149001  (after scaling by 0.9854)
G4  Ee =  -309.790329  (total electronic energy)
G4  U0 =  -309.641328  (Zero-kelvin internal energy)
G4  UT =  -309.635246  (Internal energy at 298.15 K)
G4  HT =  -309.634302  (Enthalpy at 298.15 K)
G4  GT =  -309.670957  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.496567    0.048458    0.110627
C     0.663993    1.304326    0.056958
C    -0.663991    1.304326   -0.056958
C    -1.496567    0.048459   -0.110627
C    -0.697584   -1.191548    0.318571
C     0.697583   -1.191548   -0.318571
H     1.243594   -2.103839   -0.055345
H     0.592460   -1.191190   -1.411365
H    -0.592461   -1.191190    1.411365
H    -1.243595   -2.103838    0.055345
H    -2.383763    0.165628    0.524806
H    -1.887300   -0.088226   -1.130522
H    -1.198408    2.250210   -0.113053
H     1.198410    2.250209    0.113052
H     1.887299   -0.088228    1.130522
H     2.383763    0.165626   -0.524806

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    164.3551    274.4374    399.1237    452.8988    498.4860    656.5412    731.4133
    822.3202    829.0124    884.1738    911.9663    934.6902   1006.9981   1015.7470
   1048.8786   1074.3297   1095.6292   1154.0997   1159.2438   1248.1094   1267.5771
   1291.6335   1350.8620   1368.3638   1372.9315   1385.6296   1420.4702   1472.2368
   1478.7798   1489.6274   1499.6733   1725.4484   2992.5294   2992.5299   3016.5594
   3020.7798   3037.6699   3037.9018   3067.0198   3071.1577   3135.2705   3159.6167


== Thermochemistry energies (hartree) ==
  ZPVE =     0.143712  (after scaling by 0.9854)
G4  Ee =  -234.600092  (total electronic energy)
G4  U0 =  -234.456380  (Zero-kelvin internal energy)
G4  UT =  -234.450783  (Internal energy at 298.15 K)
G4  HT =  -234.449838  (Enthalpy at 298.15 K)
G4  GT =  -234.485077  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.302792    0.943953    0.315536
C     0.616850   -0.435926   -0.258544
C    -0.419176   -1.456271    0.193451
C    -1.801222   -0.943723   -0.269860
C    -2.109924    0.489802    0.205692
C    -0.994909    1.507281   -0.183213
H    -1.218148    2.487511    0.248737
H    -0.974985    1.621016   -1.274564
H    -2.219445    0.494688    1.297537
H    -3.068213    0.821723   -0.208538
H    -2.583102   -1.623704    0.083805
H    -1.839340   -0.974565   -1.366814
H    -0.387778   -1.551912    1.285115
H    -0.211630   -2.443524   -0.232851
H     0.626240   -0.371486   -1.357767
O     1.939680   -0.675251    0.203231
O     2.597055    0.514888   -0.187848
H     1.607798    1.231593   -0.022890
H     0.408267    0.960873    1.406807

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2188.1095    155.6455    211.4014    286.6950    316.7592    335.7143    395.0762
    466.9775    508.7440    579.1339    662.9425    798.1291    821.5830    836.8471
    891.8465    915.2982    932.1422    952.8413    976.9792   1040.7711   1054.8256
   1057.2710   1100.1932   1146.0059   1167.9037   1186.7957   1194.2714   1258.5894
   1264.7888   1303.8040   1333.7004   1341.3383   1361.0695   1373.8065   1384.2603
   1393.5761   1483.5692   1486.3160   1492.3706   1501.4088   1755.0133   2983.3853
   3022.3701   3025.7877   3028.2142   3036.6024   3060.5468   3071.3737   3075.2827
   3084.6733   3088.6835

== Thermochemistry energies (hartree) ==
  ZPVE =     0.157600  (after scaling by 0.9854)
G4  Ee =  -385.446584  (total electronic energy)
G4  U0 =  -385.288984  (Zero-kelvin internal energy)
G4  UT =  -385.281823  (Internal energy at 298.15 K)
G4  HT =  -385.280879  (Enthalpy at 298.15 K)
G4  GT =  -385.320735  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.371981    0.373737    1.053040
C    -0.161629   -0.981626    0.794244
C     1.043101   -1.448515   -0.040520
C     2.039084   -0.316635   -0.339783
C     1.310314    0.977258   -0.723910
C     0.456413    1.468771    0.450758
H    -0.183006    2.308704    0.159870
H     1.114735    1.854885    1.246406
H     0.664518    0.795180   -1.592039
H     2.024148    1.754135   -1.015934
H     2.726142   -0.626168   -1.134249
H     2.653724   -0.124579    0.550092
H     0.696347   -1.881284   -0.987740
H     1.552127   -2.261160    0.488585
H    -0.497181   -1.673577    1.568313
O    -2.196038   -0.614082   -0.711407
O    -2.104545    0.594059   -0.326196
H    -1.029363    0.656650    1.869097
H    -1.209340   -1.080553   -0.014554

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -989.1772     81.9114    121.3244    195.3015    217.7750    306.9328    395.6696
    439.9946    466.0221    542.6705    650.5375    712.0307    797.3874    817.0991
    828.7140    885.6003    908.3471    945.2262    973.4392   1024.8918   1051.0477
   1074.5486   1104.6098   1145.2367   1177.0516   1233.1097   1272.5371   1279.5852
   1301.2561   1345.1781   1350.7295   1369.2102   1373.6195   1384.2669   1402.5563
   1457.3903   1486.9099   1491.9910   1502.9339   1562.0886   1594.5381   2979.5507
   3014.0804   3019.7621   3031.5543   3061.7641   3066.0464   3072.4339   3078.7084
   3105.1472   3179.7989

== Thermochemistry energies (hartree) ==
  ZPVE =     0.156874  (after scaling by 0.9854)
G4  Ee =  -385.453648  (total electronic energy)
G4  U0 =  -385.296774  (Zero-kelvin internal energy)
G4  UT =  -385.288896  (Internal energy at 298.15 K)
G4  HT =  -385.287952  (Enthalpy at 298.15 K)
G4  GT =  -385.329858  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.031170    0.960763    0.877397
C    -0.433143   -0.367343    0.823206
C     0.511085   -1.444760    0.324830
C     1.881814   -0.897391   -0.108252
C     1.727137    0.436935   -0.846571
C     1.130908    1.493072    0.095067
H     0.826779    2.387141   -0.467200
H     1.904996    1.849482    0.795032
H     1.056510    0.299590   -1.703457
H     2.689205    0.781645   -1.239316
H     2.392746   -1.634392   -0.736301
H     2.516978   -0.744815    0.774447
H     0.024008   -1.958506   -0.512219
H     0.634641   -2.198421    1.111118
H    -1.197133   -0.687070    1.523731
O    -1.637469   -0.382223   -0.642978
O    -2.870541    0.147313   -0.267943
H    -2.862789    1.024351   -0.679416
H    -0.641643    1.672628    1.426885

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -495.6700     54.8591     91.1244    142.6827    196.6286    284.6752    333.3823
    357.1983    411.8690    456.3250    496.3285    673.1680    720.0728    807.5451
    822.2060    883.8948    891.3085    910.5274    966.5961   1008.5716   1052.3155
   1058.9557   1068.9296   1081.3643   1150.0009   1155.7211   1223.3687   1260.4028
   1291.6205   1348.5340   1365.5868   1369.2063   1384.4228   1393.4459   1415.0355
   1456.6737   1473.5995   1490.5356   1499.7581   1508.1493   2968.9262   3011.6928
   3017.8528   3032.2314   3035.7349   3062.0256   3074.8652   3079.9426   3154.8761
   3178.7325   3711.4136

== Thermochemistry energies (hartree) ==
  ZPVE =     0.159130  (after scaling by 0.9854)
G4  Ee =  -385.456690  (total electronic energy)
G4  U0 =  -385.297560  (Zero-kelvin internal energy)
G4  UT =  -385.288989  (Internal energy at 298.15 K)
G4  HT =  -385.288045  (Enthalpy at 298.15 K)
G4  GT =  -385.331789  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.296883   -1.241493    0.724410
C     0.610917   -0.074210    0.841249
C     0.022609    1.322145    0.604890
C    -1.399493    1.309899    0.007847
C    -1.629943    0.113428   -0.923535
C    -1.511761   -1.200452   -0.135710
H    -1.537559   -2.073233   -0.801284
H    -2.391869   -1.315061    0.522237
H    -0.886213    0.117632   -1.726489
H    -2.619060    0.172934   -1.388837
H    -1.584689    2.249634   -0.522136
H    -2.138704    1.265311    0.819396
H     0.722634    1.832027   -0.063342
H     0.025276    1.879366    1.547885
H     1.261072   -0.100385    1.723920
O     1.244811   -0.639109   -0.282351
O     2.648056    0.292271   -0.652787
H     3.245392   -0.462701   -0.557638
H    -0.011902   -2.166724    1.212479

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -710.1189     69.9850    121.5125    138.6569    158.6698    266.3644    290.7358
    378.4804    402.9815    453.9837    519.7238    654.4903    700.0027    801.0424
    815.3820    853.1154    873.5177    890.4316    962.7115    995.7459   1008.1338
   1049.8462   1057.9790   1081.5952   1133.4225   1169.7490   1198.5625   1256.8079
   1287.5063   1302.8827   1352.2274   1358.8380   1362.5813   1386.9764   1403.0044
   1414.2931   1453.0613   1479.9731   1488.9918   1500.5256   2951.3661   3012.0321
   3023.2625   3027.3696   3048.1806   3050.5193   3069.9860   3094.0176   3100.0479
   3195.9491   3785.5190

== Thermochemistry energies (hartree) ==
  ZPVE =     0.158160  (after scaling by 0.9854)
G4  Ee =  -385.460406  (total electronic energy)
G4  U0 =  -385.302246  (Zero-kelvin internal energy)
G4  UT =  -385.293592  (Internal energy at 298.15 K)
G4  HT =  -385.292648  (Enthalpy at 298.15 K)
G4  GT =  -385.336209  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 7: α-cyclohexenyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.273160   -0.672737    0.196088
C    -1.215134    0.816055    0.003182
C     0.000578    1.475157   -0.092136
C     1.215775    0.815105    0.003172
C     1.272629   -0.673728    0.196097
C    -0.000530   -1.358445   -0.330381
H    -0.000945   -2.420453   -0.063881
H    -0.000503   -1.302193   -1.425598
H     1.399413   -0.904521    1.267224
H     2.158587   -1.090980   -0.297734
H     2.145263    1.373631   -0.036896
H     0.000998    2.553494   -0.231821
H    -2.144185    1.375309   -0.036876
H    -2.159438   -1.089286   -0.297763
H    -1.400142   -0.903443    1.267210

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    183.1543    252.2057    429.1736    501.4861    512.1960    608.5259    690.2600
    725.1101    836.5046    858.6848    892.5188    956.2417    966.1075   1011.6685
   1058.1975   1062.2706   1139.1646   1139.8501   1158.7638   1222.0980   1268.1305
   1343.9785   1354.2579   1367.9151   1401.0833   1444.4631   1472.1294   1475.2390
   1491.1251   1510.4595   2962.7618   2964.4056   3027.3107   3040.8421   3047.9702
   3076.2769   3149.1289   3176.2056   3185.6391

== Thermochemistry energies (hartree) ==
  ZPVE =     0.130123  (after scaling by 0.9854)
G4  Ee =  -233.955349  (total electronic energy)
G4  U0 =  -233.825226  (Zero-kelvin internal energy)
G4  UT =  -233.819639  (Internal energy at 298.15 K)
G4  HT =  -233.818694  (Enthalpy at 298.15 K)
G4  GT =  -233.854462  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.135753   -0.317973   -0.252972
C    -1.636443    1.094855   -0.116558
C    -0.387762    1.413113    0.227156
C     0.646764    0.379947    0.555579
C     0.075062   -1.023769    0.736691
C    -0.985385   -1.330997   -0.325337
H    -1.365325   -2.349917   -0.204260
H    -0.519488   -1.277928   -1.316173
H    -0.365934   -1.082286    1.739876
H     0.902735   -1.737969    0.706041
H    -0.079076    2.452413    0.288855
H    -2.354037    1.890280   -0.305652
H    -2.772704   -0.395767   -1.142343
H    -2.795724   -0.546863    0.597936
O     1.611812    0.382763   -0.577345
H     1.245799    0.671182    1.423127
O     2.718795   -0.247037   -0.264500

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     77.5627    112.1541    214.5211    264.9722    341.6828    435.4363    454.9981
    530.2659    565.0153    697.5004    737.7540    827.7007    836.4692    888.5017
    905.3452    946.0548   1013.2325   1014.4950   1065.3168   1073.1519   1108.6502
   1156.7182   1175.4341   1204.9659   1259.8687   1276.4635   1324.8282   1349.6045
   1362.7533   1374.6094   1392.3402   1425.1099   1468.1559   1481.6496   1494.6014
   1717.4831   2995.7392   3031.2909   3038.9523   3051.9343   3070.9059   3086.5341
   3095.1382   3148.3292   3177.3420

== Thermochemistry energies (hartree) ==
  ZPVE =     0.139794  (after scaling by 0.9854)
G4  Ee =  -384.277970  (total electronic energy)
G4  U0 =  -384.138176  (Zero-kelvin internal energy)
G4  UT =  -384.130668  (Internal energy at 298.15 K)
G4  HT =  -384.129724  (Enthalpy at 298.15 K)
G4  GT =  -384.170916  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.273428   -0.273578   -0.081416
C    -1.685730    1.111594   -0.086247
C    -0.401163    1.374668    0.150694
C     0.609508    0.315808    0.493961
C     0.029942   -1.056561    0.528790
C    -1.192060   -1.356259   -0.273078
H    -1.590702   -2.346746   -0.033529
H    -0.927954   -1.380643   -1.345323
H     0.616615   -1.856555    0.966621
H    -0.025353    2.392842    0.121430
H    -2.368991    1.934799   -0.282542
H    -3.033618   -0.357982   -0.866771
H    -2.804721   -0.439057    0.866923
O     1.640509    0.453200   -0.532073
H     1.100712    0.557645    1.446103
O     2.823342   -0.224124   -0.053233
H     2.800781   -1.030944   -0.586691

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     62.3684    116.2947    173.0854    243.8703    248.4454    295.7343    375.1969
    450.7767    499.4854    548.5989    582.4250    720.6364    755.0868    840.2029
    885.0535    913.6300    935.2001    962.3924    984.3945   1005.5061   1029.8747
   1065.8585   1125.9299   1170.2998   1180.4905   1268.2127   1308.0636   1317.2320
   1346.4491   1370.9528   1378.7243   1396.9286   1421.5023   1464.2831   1477.8900
   1721.7701   2940.9632   3006.8324   3010.7689   3052.6253   3071.7526   3148.6364
   3180.9428   3187.7191   3752.6996

== Thermochemistry energies (hartree) ==
  ZPVE =     0.136930  (after scaling by 0.9854)
G4  Ee =  -384.251883  (total electronic energy)
G4  U0 =  -384.114953  (Zero-kelvin internal energy)
G4  UT =  -384.106572  (Internal energy at 298.15 K)
G4  HT =  -384.105628  (Enthalpy at 298.15 K)
G4  GT =  -384.148565  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.608883   -0.557352    0.103327
C    -1.373107    0.914532   -0.129827
C    -0.176861    1.489547   -0.002002
C     1.015302    0.700960    0.401441
C     0.930954   -0.765582    0.363500
C    -0.353092   -1.422207   -0.130407
H    -0.481656   -2.399073    0.346441
H    -0.231288   -1.602736   -1.203464
H    -0.047681    2.554857   -0.170143
H    -2.237760    1.518282   -0.394587
H    -2.419709   -0.910035   -0.543484
H    -1.977819   -0.694798    1.130708
O     1.694226   -0.057708   -0.621093
H     1.694713    1.177008    1.108444
H     1.541504   -1.341230    1.058640

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    112.3600    248.8496    393.9407    480.0332    502.2682    538.5923    718.7188
    757.5524    793.3936    827.6060    871.7301    940.6470    968.2761    971.3757
   1000.3862   1048.8250   1060.8853   1088.5392   1148.8997   1193.6130   1213.0527
   1270.9291   1288.9269   1346.6484   1350.5963   1392.5185   1420.8799   1460.3077
   1475.2179   1483.3434   1712.9928   2999.7058   3043.4451   3059.8529   3087.3913
   3102.9364   3114.8272   3150.5975   3175.8273

== Thermochemistry energies (hartree) ==
  ZPVE =     0.125303  (after scaling by 0.9854)
G4  Ee =  -308.552650  (total electronic energy)
G4  U0 =  -308.427347  (Zero-kelvin internal energy)
G4  UT =  -308.421480  (Internal energy at 298.15 K)
G4  HT =  -308.420536  (Enthalpy at 298.15 K)
G4  GT =  -308.456924  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.193587    0.731170    0.239101
C     0.114871    1.422535   -0.063981
C     1.257282    0.724889   -0.104548
C     1.257282   -0.724889    0.104548
C     0.114871   -1.422535    0.063981
C    -1.193587   -0.731170   -0.239101
H    -2.033578   -1.271891    0.208930
H    -1.360159   -0.763727   -1.328383
H     0.115451   -2.501737    0.184561
H     2.206889    1.223532   -0.273961
H     0.115450    2.501737   -0.184561
H    -2.033578    1.271891   -0.208930
H    -1.360159    0.763727    1.328383
H     2.206889   -1.223532    0.273961

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    185.8733    300.8950    477.0534    520.8010    570.0290    678.5848    760.0494
    789.1189    855.3345    931.3977    964.9377    976.3344    995.8444   1007.4120
   1044.2655   1071.2778   1167.2376   1186.0426   1204.0793   1267.1456   1351.7339
   1358.6946   1399.8273   1437.0243   1467.2001   1479.0894   1648.4249   1708.6853
   2967.9427   2979.5188   3065.1647   3065.3860   3156.2752   3163.3752   3178.6951
   3188.1616

== Thermochemistry energies (hartree) ==
  ZPVE =     0.120257  (after scaling by 0.9854)
G4  Ee =  -233.369786  (total electronic energy)
G4  U0 =  -233.249529  (Zero-kelvin internal energy)
G4  UT =  -233.244268  (Internal energy at 298.15 K)
G4  HT =  -233.243324  (Enthalpy at 298.15 K)
G4  GT =  -233.277832  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.029311   -0.580924   -0.160666
C    -1.770116    0.901695   -0.143499
C    -0.588200    1.452318    0.138952
C     0.609450    0.630778    0.512550
C     0.294050   -0.855574    0.723405
C    -0.717259   -1.397987   -0.251469
H    -0.916120   -2.459151   -0.079342
H    -0.322804   -1.288091   -1.268345
H     0.191053   -1.180661    1.759529
H     1.585228   -1.085551    0.296613
H    -0.464050    2.531359    0.132649
H    -2.615960    1.546629   -0.371216
H    -2.680524   -0.833356   -1.006064
H    -2.590494   -0.863600    0.741781
O     1.551218    0.626476   -0.585074
H     1.111027    1.033232    1.402897
O     2.437651   -0.414307   -0.230443

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2157.5303    113.7017    193.0375    244.8613    288.8035    425.6294    459.3068
    520.2369    585.7889    679.2871    727.7219    743.4715    827.8693    855.1591
    883.4983    930.0590    949.6254    976.7347    990.2109   1006.8699   1050.9112
   1067.6589   1104.9266   1128.5456   1165.1860   1211.7255   1254.1253   1310.0181
   1317.3226   1345.3556   1365.3451   1388.6983   1414.9337   1471.0430   1484.9410
   1709.1981   1738.7232   3006.9139   3013.1076   3037.8701   3054.3622   3093.4991
   3120.9345   3148.4616   3175.8453

== Thermochemistry energies (hartree) ==
  ZPVE =     0.133755  (after scaling by 0.9854)
G4  Ee =  -384.218254  (total electronic energy)
G4  U0 =  -384.084499  (Zero-kelvin internal energy)
G4  UT =  -384.077509  (Internal energy at 298.15 K)
G4  HT =  -384.076564  (Enthalpy at 298.15 K)
G4  GT =  -384.116261  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.125813   -0.426875   -0.277394
C    -1.683211    1.007767   -0.412619
C    -0.542428    1.444892    0.146170
C     0.274895    0.540291    0.929437
C     0.154639   -0.843796    0.800024
C    -0.924999   -1.377063   -0.156647
H    -1.255457   -2.368273    0.165612
H    -0.487758   -1.505892   -1.155204
H     0.400156   -1.449606    1.672664
H     1.299960   -0.983329    0.127167
H    -0.249718    2.487358    0.080057
H    -2.337837    1.701766   -0.932270
H    -2.743180   -0.716172   -1.134549
H    -2.781676   -0.509970    0.603811
O     2.219907    0.647617   -0.373254
H     0.893234    0.958748    1.715493
O     2.323065   -0.608357   -0.541321

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1086.0841     97.6810    126.2665    183.9552    206.6816    295.1743    401.8751
    495.2524    525.7261    585.1267    646.2231    725.1551    759.8647    848.9078
    851.9709    925.8987    962.1401    989.0995    993.7571   1006.3191   1057.4168
   1072.4494   1168.8122   1183.4066   1215.3850   1252.7327   1287.8540   1345.5687
   1348.6096   1364.3920   1394.4599   1429.6912   1467.8253   1487.2477   1543.5277
   1579.8116   1663.9739   2985.3807   3021.0815   3065.6802   3084.7944   3117.5590
   3165.6674   3188.2757   3201.8742

== Thermochemistry energies (hartree) ==
  ZPVE =     0.133169  (after scaling by 0.9854)
G4  Ee =  -384.222617  (total electronic energy)
G4  U0 =  -384.089448  (Zero-kelvin internal energy)
G4  UT =  -384.081770  (Internal energy at 298.15 K)
G4  HT =  -384.080826  (Enthalpy at 298.15 K)
G4  GT =  -384.122315  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.304975   -0.186164   -0.207918
C    -1.650033    1.170480   -0.162011
C    -0.398735    1.347291    0.273827
C     0.421700    0.215002    0.731160
C    -0.098096   -1.070550    0.623498
C    -1.270257   -1.326000   -0.276705
H    -1.740590   -2.287062   -0.047047
H    -0.901025   -1.403050   -1.312978
H     0.429267   -1.908105    1.067993
H     3.134186   -0.972580   -0.411684
H     0.048867    2.334367    0.309164
H    -2.247366    2.027108   -0.462808
H    -2.985553   -0.249556   -1.063874
H    -2.938209   -0.304362    0.685147
O     1.740383    0.243428   -0.655075
H     1.173401    0.416388    1.485983
O     2.988291   -0.062616   -0.112550

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -489.7085     61.7480     92.2428    155.3747    206.4314    262.5798    327.1685
    407.4387    484.6277    491.0781    566.2647    678.5967    738.5538    767.8904
    852.7393    923.6038    956.6543    964.0701    995.2985    997.0836   1027.8873
   1045.5591   1071.6622   1162.7303   1179.5664   1188.5256   1268.2578   1336.8422
   1351.1400   1387.4520   1401.2181   1433.8907   1460.7432   1476.6804   1488.1833
   1696.9456   2966.2767   2990.8861   3060.5313   3071.4172   3159.8160   3174.1093
   3187.6202   3197.8091   3709.6010

== Thermochemistry energies (hartree) ==
  ZPVE =     0.135648  (after scaling by 0.9854)
G4  Ee =  -384.225841  (total electronic energy)
G4  U0 =  -384.090193  (Zero-kelvin internal energy)
G4  UT =  -384.081922  (Internal energy at 298.15 K)
G4  HT =  -384.080978  (Enthalpy at 298.15 K)
G4  GT =  -384.124061  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.222152    0.155064   -0.228172
C    -1.327132    1.361334   -0.092324
C    -0.060795    1.298496    0.316241
C     0.585830    0.006464    0.717691
C    -0.255484   -1.197271    0.557460
C    -1.422798   -1.159453   -0.369414
H    -2.067158   -2.030223   -0.213305
H    -1.046674   -1.229683   -1.399794
H     0.031474   -2.104980    1.071803
H     3.418715   -0.399723   -0.299127
H     0.559076    2.186945    0.375156
H    -1.764141    2.323542   -0.348572
H    -2.876620    0.275792   -1.098647
H    -2.894031    0.094028    0.639833
O     1.380133   -0.606423   -0.266098
H     1.110263    0.089335    1.678205
O     2.837903    0.357317   -0.460707

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -721.7624     77.5931    123.7023    154.2163    173.7788    262.5231    284.7243
    392.0086    485.9008    513.7788    543.4080    670.6914    738.1378    757.4259
    838.7102    891.0157    934.8442    941.0039    978.9102   1000.7853   1017.5373
   1021.9513   1063.9259   1136.5106   1175.7944   1180.6070   1264.5772   1278.9225
   1320.7943   1348.9755   1393.6695   1410.4399   1420.7233   1457.3250   1481.4111
   1719.4512   3005.7456   3012.4550   3019.7124   3058.7862   3075.9398   3152.0346
   3191.1983   3219.7989   3783.1817

== Thermochemistry energies (hartree) ==
  ZPVE =     0.134637  (after scaling by 0.9854)
G4  Ee =  -384.225917  (total electronic energy)
G4  U0 =  -384.091280  (Zero-kelvin internal energy)
G4  UT =  -384.082937  (Internal energy at 298.15 K)
G4  HT =  -384.081993  (Enthalpy at 298.15 K)
G4  GT =  -384.124864  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 8: β-cyclohexenyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.484399   -0.339764   -0.017358
C     0.397376   -1.350276   -0.188920
C    -0.988040   -1.026382    0.262331
C    -1.422367    0.385008   -0.186836
C    -0.320752    1.396689   -0.002155
C     0.968601    1.072861    0.086612
H    -2.314273    0.695187    0.371166
H    -1.725409    0.361980   -1.243654
H    -1.039909   -1.056022    1.366622
H    -1.701923   -1.777849   -0.091092
H     0.665800   -2.373223   -0.431459
H     2.204661   -0.407227   -0.848378
H     2.096247   -0.565592    0.878271
H     1.714862    1.851657    0.224962
H    -0.615358    2.442267    0.051518

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    135.8948    202.7595    383.0498    391.9995    493.7646    536.5584    670.5163
    751.5001    830.6440    885.3598    907.8928    922.4173    980.8747   1001.8238
   1027.6276   1048.8244   1115.5755   1163.3498   1174.6693   1191.7075   1269.1596
   1321.2125   1344.4407   1361.9066   1394.3696   1422.7514   1450.9133   1468.0807
   1482.1043   1726.3158   2903.0973   2921.9393   2981.4592   3002.6153   3043.5694
   3060.8381   3139.3092   3163.4042   3176.9746

== Thermochemistry energies (hartree) ==
  ZPVE =     0.128973  (after scaling by 0.9854)
G4  Ee =  -233.931708  (total electronic energy)
G4  U0 =  -233.802735  (Zero-kelvin internal energy)
G4  UT =  -233.796797  (Internal energy at 298.15 K)
G4  HT =  -233.795853  (Enthalpy at 298.15 K)
G4  GT =  -233.832429  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -233.616222730409  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.152726    1.211045    0.715029
C     0.644944   -0.234998    0.709209
C    -0.492805   -1.248930    0.748155
C    -1.485174   -1.038293   -0.406861
C    -1.818702    0.416208   -0.609908
C    -1.093775    1.413237   -0.105601
H    -2.400240   -1.609846   -0.211679
H    -1.070289   -1.451431   -1.336145
H    -1.007838   -1.120589    1.707121
H    -0.087544   -2.265253    0.732580
H     1.368541   -0.400691    1.511849
H     0.969560    1.845735    0.353119
H    -0.021792    1.518306    1.755890
H    -1.390616    2.443533   -0.284603
H    -2.694664    0.639727   -1.213719
O     1.374918   -0.514533   -0.540481
O     2.486532    0.175895   -0.623837

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     84.7786    132.0081    161.0668    306.0157    339.5836    395.6313    466.1165
    546.5699    585.5990    673.2585    758.6653    821.5192    842.9222    891.5528
    915.5459    955.4948   1001.9785   1006.0232   1047.2705   1061.8787   1103.2898
   1160.6413   1198.4280   1219.7795   1235.1522   1270.7450   1335.1701   1343.8782
   1358.8122   1373.0351   1394.1174   1422.9513   1464.8397   1474.7401   1484.3854
   1729.3692   3012.3544   3019.6702   3039.8369   3054.7225   3064.6223   3077.4407
   3089.5221   3146.4591   3169.4338

== Thermochemistry energies (hartree) ==
  ZPVE =     0.139716  (after scaling by 0.9854)
G4  Ee =  -384.278103  (total electronic energy)
G4  U0 =  -384.138387  (Zero-kelvin internal energy)
G4  UT =  -384.130885  (Internal energy at 298.15 K)
G4  HT =  -384.129941  (Enthalpy at 298.15 K)
G4  GT =  -384.171027  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.856809  (total electronic energy)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.087325    1.164726    0.607062
C     0.597779   -0.247674    0.685166
C    -0.548680   -1.264546    0.660054
C    -1.554496   -0.978655   -0.468234
C    -1.965074    0.463515   -0.492275
C    -1.144567    1.446872    0.034997
H    -2.431987   -1.627038   -0.363813
H    -1.099881   -1.244098   -1.435068
H    -1.058869   -1.207274    1.627860
H    -0.133861   -2.272143    0.564766
H     1.209597   -0.384276    1.585449
H     2.328671    0.930880   -1.063053
H     0.711237    1.961625    0.995316
H    -1.477010    2.481478   -0.004873
H    -2.905736    0.732989   -0.961474
O     1.415329   -0.599639   -0.452219
O     2.587685    0.239942   -0.435997

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     80.2347    141.5330    172.9412    267.6953    295.2575    343.4182    428.4045
    482.1086    545.2478    593.3740    653.1714    709.9026    760.1530    838.8470
    878.4016    911.5101    955.7332    967.5177    976.0116   1010.2551   1051.7958
   1086.6700   1136.7319   1161.7653   1202.0647   1234.7452   1323.7399   1347.0848
   1358.6336   1378.2698   1387.0232   1400.7005   1451.5705   1467.9828   1477.1839
   1506.2828   2991.2897   3025.0095   3044.4406   3057.0149   3095.5601   3150.5274
   3181.5297   3194.7954   3739.8022

== Thermochemistry energies (hartree) ==
  ZPVE =     0.137981  (after scaling by 0.9854)
G4  Ee =  -384.276625  (total electronic energy)
G4  U0 =  -384.138644  (Zero-kelvin internal energy)
G4  UT =  -384.130675  (Internal energy at 298.15 K)
G4  HT =  -384.129731  (Enthalpy at 298.15 K)
G4  GT =  -384.171576  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.855746  (total electronic energy)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.037122    0.781370   -0.263494
C    -1.040984   -0.691292   -0.334161
C     0.287197   -1.411554   -0.401625
C     1.407693   -0.647884    0.335344
C     1.398344    0.827163    0.027585
C     0.268854    1.485358   -0.241080
H     2.379124   -1.085690    0.083108
H     1.279328   -0.786643    1.415995
H     0.546001   -1.525627   -1.462741
H     0.192039   -2.422363    0.010113
H    -1.881217   -1.187060   -0.822810
H    -1.889669    1.329667   -0.658919
H     0.273604    2.549958   -0.453534
H     2.345861    1.358236    0.053616
O    -1.368620   -0.036180    0.887470

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    184.2735    272.9549    352.5473    469.9996    511.0246    638.3203    701.6634
    723.2301    807.1387    825.2455    870.5349    941.5471    943.3760    984.9963
    992.5077   1043.3894   1057.6566   1084.6237   1139.1559   1189.6818   1212.6117
   1266.9436   1279.9545   1342.4273   1356.7165   1389.1101   1422.1095   1455.6735
   1475.5635   1485.2511   1706.7477   3023.2285   3030.7340   3065.7167   3073.6136
   3096.4340   3130.9455   3158.6298   3183.3470

== Thermochemistry energies (hartree) ==
  ZPVE =     0.125467  (after scaling by 0.9854)
G4  Ee =  -308.558055  (total electronic energy)
G4  U0 =  -308.432588  (Zero-kelvin internal energy)
G4  UT =  -308.426868  (Internal energy at 298.15 K)
G4  HT =  -308.425924  (Enthalpy at 298.15 K)
G4  GT =  -308.461770  (Gibbs free energy at 298.15 K)
```

Species 5: alkene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.047524    0.730845    1.257280
C     0.047524    1.423185    0.114882
C     0.295564    0.710221   -1.193586
C    -0.295564   -0.710221   -1.193586
C    -0.047524   -1.423185    0.114882
C     0.047524   -0.730845    1.257280
H     0.108843   -1.284331   -2.033557
H    -1.384043   -0.657496   -1.360242
H     1.384043    0.657496   -1.360242
H    -0.108843    1.284331   -2.033557
H     0.011746    2.508512    0.115458
H    -0.177426    1.241201    2.206890
H     0.177426   -1.241201    2.206890
H    -0.011746   -2.508512    0.115458

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    186.0290    301.2623    477.1317    520.7165    570.0125    678.6001    760.0196
    789.1127    855.3562    931.7446    965.0870    976.3074    995.7907   1007.4493
   1044.4666   1071.5700   1167.2195   1186.0940   1204.0624   1267.2125   1351.7886
   1358.8273   1399.9285   1437.0354   1467.3006   1479.1517   1648.4474   1708.7140
   2967.9538   2979.5330   3065.0911   3065.3062   3156.2296   3163.3576   3178.6748
   3188.1131

== Thermochemistry energies (hartree) ==
  ZPVE =     0.120261  (after scaling by 0.9854)
G4  Ee =  -233.369786  (total electronic energy)
G4  U0 =  -233.249525  (Zero-kelvin internal energy)
G4  UT =  -233.244265  (Internal energy at 298.15 K)
G4  HT =  -233.243320  (Enthalpy at 298.15 K)
G4  GT =  -233.277172  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.376310    1.048705    0.686059
C     0.619052   -0.474741    0.695945
C    -0.653686   -1.308780    0.622955
C    -1.585412   -0.826630   -0.501670
C    -1.756032    0.666216   -0.482693
C    -0.869167    1.500257    0.109490
H    -2.563118   -1.313817   -0.412028
H    -1.183764   -1.136866   -1.475292
H    -1.166409   -1.225658    1.588086
H    -0.392731   -2.362861    0.484989
H     1.233240   -0.737328    1.566571
H     1.417161    1.156839   -0.129004
H     0.731951    1.608867    1.552532
H    -1.084932    2.565342    0.145307
H    -2.650455    1.076994   -0.942950
O     1.363092   -0.740051   -0.510550
O     2.245991    0.332341   -0.634291

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2223.9678    114.1516    166.9165    250.4323    337.9654    406.7149    479.6986
    545.7329    605.2991    666.0178    707.4598    777.8104    815.4433    861.8204
    876.9721    941.8802    949.0178    962.3108    999.5188   1013.2690   1056.7024
   1081.6784   1107.8901   1179.7953   1200.9488   1217.8017   1254.1000   1304.2326
   1331.1683   1357.7221   1376.0048   1391.5496   1444.0362   1466.3002   1477.6857
   1603.8653   1708.6512   3021.7561   3023.6021   3043.0939   3059.5722   3088.1978
   3107.3166   3151.4481   3173.7032

== Thermochemistry energies (hartree) ==
  ZPVE =     0.134037  (after scaling by 0.9854)
G4  Ee =  -384.227010  (total electronic energy)
G4  U0 =  -384.092973  (Zero-kelvin internal energy)
G4  UT =  -384.086042  (Internal energy at 298.15 K)
G4  HT =  -384.085098  (Enthalpy at 298.15 K)
G4  GT =  -384.124705  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -383.807209  (total electronic energy)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.134716    1.018022    0.836328
C     0.355361   -0.339787    1.090460
C    -0.598551   -1.378106    0.579168
C    -1.333436   -0.938721   -0.699752
C    -1.794186    0.497457   -0.608679
C    -1.106838    1.392011    0.104837
H    -2.179515   -1.608328   -0.884749
H    -0.660222   -1.054673   -1.561082
H    -1.333692   -1.544294    1.384871
H    -0.089286   -2.334186    0.427556
H     1.040993   -0.637025    1.876581
H     1.125965    1.092919   -0.095180
H     0.521347    1.734874    1.559974
H    -1.419831    2.430617    0.149167
H    -2.679697    0.792290   -1.162968
O     1.938830   -0.618796   -0.373597
O     2.027612    0.571614   -0.814945

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1074.8556    107.5879    132.7030    202.7679    233.2763    378.9131    421.1442
    488.3301    542.5577    599.9634    632.4915    722.4215    763.4658    834.2065
    871.4635    937.0488    949.3748    958.3882    991.7348   1020.9491   1046.7081
   1067.2259   1155.5456   1180.7518   1204.3982   1251.7335   1265.4012   1341.9732
   1348.6922   1355.4842   1396.4578   1420.8283   1456.8639   1483.8953   1519.0882
   1605.1333   1703.8313   2972.1232   3008.6438   3068.1881   3080.2169   3124.2232
   3164.2465   3185.9172   3189.3299

== Thermochemistry energies (hartree) ==
  ZPVE =     0.133315  (after scaling by 0.9854)
G4  Ee =  -384.227801  (total electronic energy)
G4  U0 =  -384.094486  (Zero-kelvin internal energy)
G4  UT =  -384.087022  (Internal energy at 298.15 K)
G4  HT =  -384.086078  (Enthalpy at 298.15 K)
G4  GT =  -384.126929  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.151275    1.214466    0.639751
C     0.312582   -0.036335    0.980894
C    -0.576145   -1.232640    0.755849
C    -1.442891   -1.080324   -0.507291
C    -2.007045    0.309028   -0.646303
C    -1.364350    1.373743   -0.117978
H    -2.243877   -1.827032   -0.506910
H    -0.828994   -1.292232   -1.395291
H    -1.224675   -1.338139    1.639380
H     0.026908   -2.141970    0.696551
H     1.110044   -0.129221    1.707642
H     2.723435    0.904290   -1.072854
H     0.404699    2.097819    0.937207
H    -1.750250    2.377010   -0.272967
H    -2.906348    0.446270   -1.239225
O     1.680268   -0.523241   -0.503050
O     2.827707    0.225188   -0.387333

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -379.9481     30.4483    104.6119    119.4758    197.0658    276.7852    307.5545
    413.8166    484.0201    512.7977    574.7142    687.5744    758.0977    817.3025
    855.7204    924.6059    942.8683    977.6288    984.7231    996.2287   1008.9077
   1041.6975   1076.8221   1166.4118   1179.4231   1193.7162   1265.3625   1347.7210
   1356.9303   1404.9280   1405.5332   1445.9061   1463.1146   1472.8391   1479.9961
   1627.4317   2988.6681   3003.5282   3064.2084   3093.7637   3159.4327   3174.2188
   3185.3988   3204.9776   3680.6197   -379.9481     30.4476    104.6119    119.4759
    197.0660    276.7853    307.5545    413.8166    484.0201    512.7977    574.7142
    687.5744    758.0977    817.3026    855.7204    924.6059    942.8683    977.6288
    984.7231    996.2287   1008.9076   1041.6974   1076.8220   1166.4118   1179.4230
   1193.7161   1265.3624   1347.7209   1356.9302   1404.9280   1405.5331   1445.9060
   1463.1144   1472.8389   1479.9960   1627.4318   2988.6681   3003.5282   3064.2084
   3093.7637   3159.4327   3174.2188   3185.3987   3204.9776   3680.6197

== Thermochemistry energies (hartree) ==
  ZPVE =     0.135722  (after scaling by 0.9854)
G4  Ee =  -384.231876  (total electronic energy)
G4  U0 =  -384.096154  (Zero-kelvin internal energy)
G4  UT =  -384.087809  (Internal energy at 298.15 K)
G4  HT =  -384.086865  (Enthalpy at 298.15 K)
G4  GT =  -384.130717  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.453615   -1.367349    0.409385
C    -0.527091   -0.328385    0.812296
C     0.031343    1.085269    0.907151
C     0.973221    1.401925   -0.266943
C     1.937121    0.290840   -0.551276
C     1.656225   -1.005691   -0.249930
H     1.510938    2.339579   -0.090222
H     0.367375    1.562331   -1.170092
H     0.569911    1.175620    1.858973
H    -0.802077    1.791756    0.927843
H    -1.149890   -0.585737    1.678000
H    -3.143933   -0.444094   -0.828721
H     0.218216   -2.403966    0.610852
H     2.351056   -1.792363   -0.528237
H     2.862276    0.532483   -1.067018
O    -1.099482   -0.668860   -0.406610
O    -2.641827    0.339452   -0.562825

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -643.7137     68.5795    126.8522    142.1841    208.7457    236.3302    314.6104
    374.5625    477.2465    528.6246    599.2069    682.1976    748.9355    813.8973
    836.0285    866.3055    908.4730    926.5510    977.0548    985.4077    999.0855
   1061.9316   1096.1606   1144.6528   1183.0960   1196.6620   1259.7733   1286.7329
   1335.9251   1360.1286   1396.1529   1419.0037   1445.9152   1455.5111   1478.3167
   1574.9260   3015.3118   3022.8025   3037.8906   3067.1834   3104.8123   3161.8998
   3181.2885   3223.8621   3783.9535

== Thermochemistry energies (hartree) ==
  ZPVE =     0.134952  (after scaling by 0.9854)
G4  Ee =  -384.243986  (total electronic energy)
G4  U0 =  -384.109034  (Zero-kelvin internal energy)
G4  UT =  -384.100753  (Internal energy at 298.15 K)
G4  HT =  -384.099809  (Enthalpy at 298.15 K)
G4  GT =  -384.142593  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 9: cyclohexadienyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.739991   -1.223502   -0.000038
C     1.453654    0.000001   -0.000065
C     0.739989    1.223503   -0.000028
C    -0.622331    1.254147    0.000033
C    -1.447519   -0.000001    0.000065
C    -0.622329   -1.254148    0.000023
H    -2.137853    0.000002   -0.864876
H    -2.137776   -0.000006    0.865068
H    -1.151043    2.202331    0.000061
H     1.295920    2.156770   -0.000049
H     2.537129    0.000002   -0.000114
H    -1.151039   -2.202333    0.000043
H     1.295924   -2.156767   -0.000067

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    182.6707    384.9461    530.5428    561.1570    588.9585    646.0198    733.4097
    773.7465    872.4882    936.8705    968.3608    969.2326    980.0754    987.2943
    993.9733   1114.4403   1166.6864   1171.7547   1198.9860   1309.2668   1360.3413
   1408.9065   1435.9745   1454.9387   1544.4797   1610.3738   2905.9071   2918.6092
   3158.3743   3160.3792   3179.1297   3180.0507   3202.8703

== Thermochemistry energies (hartree) ==
  ZPVE =     0.106838  (after scaling by 0.9854)
G4  Ee =  -232.737066  (total electronic energy)
G4  U0 =  -232.630228  (Zero-kelvin internal energy)
G4  UT =  -232.625114  (Internal energy at 298.15 K)
G4  HT =  -232.624170  (Enthalpy at 298.15 K)
G4  GT =  -232.659004  (Gibbs free energy at 298.15 K)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.946071    0.366753   -0.521657
C     1.652862   -1.016761   -0.157044
C     0.488296   -1.370240    0.406502
C    -0.584308   -0.348138    0.614601
C    -0.068987    1.085551    0.721912
C     1.141918    1.361002   -0.124033
H     0.180828    1.285600    1.775366
H    -0.900237    1.756520    0.481247
H     0.268320   -2.402310    0.655118
H     2.410481   -1.769431   -0.354919
O    -1.483356   -0.468771   -0.583038
H    -1.235267   -0.584020    1.458794
O    -2.565433    0.253708   -0.441339
H     1.370027    2.395194   -0.362023
H     2.841039    0.569948   -1.100238

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     78.9669    124.4064    209.8113    313.5798    378.6430    470.4839    511.8397
    590.4836    611.1580    670.0181    787.0555    806.6984    852.8027    951.1396
    964.5550    977.6224    989.2602   1000.9962   1009.3982   1101.7329   1171.7363
   1205.8211   1206.9190   1215.7556   1319.1811   1337.6998   1355.8018   1409.6011
   1442.4400   1450.8066   1640.2591   1710.7435   2997.4347   3076.6886   3091.5821
   3165.9573   3174.0595   3192.3142   3198.8966

== Thermochemistry energies (hartree) ==
  ZPVE =     0.116206  (after scaling by 0.9854)
G4  Ee =  -383.046297  (total electronic energy)
G4  U0 =  -382.930091  (Zero-kelvin internal energy)
G4  UT =  -382.922921  (Internal energy at 298.15 K)
G4  HT =  -382.921977  (Enthalpy at 298.15 K)
G4  GT =  -382.962447  (Gibbs free energy at 298.15 K)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.225941    0.304246   -0.235867
C     1.782209   -1.031978   -0.094343
C     0.490669   -1.321029    0.231339
C    -0.527426   -0.248381    0.460862
C     0.016149    1.138281    0.294811
C     1.316396    1.371198   -0.040757
H    -0.680159    1.955671    0.447822
H     0.145499   -2.344878    0.322887
H     2.488942   -1.841832   -0.248322
O    -1.602422   -0.531515   -0.480441
H    -0.979838   -0.360679    1.460952
O    -2.759467    0.225051   -0.050235
H    -2.826470    0.868427   -0.769506
H     3.256300    0.509139   -0.502085
H     1.667209    2.391836   -0.162617

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     80.6606    123.4032    230.7530    259.0123    369.6007    382.8152    451.5817
    564.3703    583.6103    621.0640    690.7445    758.2268    810.5953    882.7285
    924.2795    929.9278    963.7857    977.7121    994.4166   1003.0443   1040.8364
   1124.1904   1162.5861   1192.9556   1299.1507   1315.9314   1349.2404   1375.5684
   1409.2601   1448.5617   1542.9318   1597.0315   2943.0869   3164.6466   3170.0165
   3190.9943   3194.9566   3204.2555   3759.3203

== Thermochemistry energies (hartree) ==
  ZPVE =     0.114687  (after scaling by 0.9854)
G4  Ee =  -383.055369  (total electronic energy)
G4  U0 =  -382.940682  (Zero-kelvin internal energy)
G4  UT =  -382.933138  (Internal energy at 298.15 K)
G4  HT =  -382.932194  (Enthalpy at 298.15 K)
G4  GT =  -382.973274  (Gibbs free energy at 298.15 K)
```

Species 4: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.262383    1.416858   -0.723505
C    -0.262383    1.416858    0.723505
C    -0.262383    0.266294    1.430151
C    -0.048925   -1.020134    0.759443
C    -0.048925   -1.020134   -0.759443
C    -0.262383    0.266294   -1.430151
H    -0.444533    0.265464    2.499827
H    -0.379401    2.367325    1.234586
O     1.153133   -1.170794   -0.000000
H    -0.346458   -1.927723    1.281871
H    -0.346458   -1.927723   -1.281871
H    -0.444533    0.265464   -2.499827
H    -0.379401    2.367325   -1.234586

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    253.7927    318.0619    464.7663    540.3432    616.3297    638.2910    700.1100
    782.2493    782.5579    854.4873    935.8458    963.4724    972.6337    982.0710
    985.3129   1008.5607   1057.5928   1131.8041   1187.6446   1204.6776   1259.4584
   1354.9766   1381.0430   1421.6052   1461.0299   1601.3081   1683.1944   3118.2390
   3127.6730   3165.4700   3174.6024   3187.5457   3195.3965

== Thermochemistry energies (hartree) ==
  ZPVE =     0.102171  (after scaling by 0.9854)
G4  Ee =  -307.331379  (total electronic energy)
G4  U0 =  -307.229208  (Zero-kelvin internal energy)
G4  UT =  -307.223966  (Internal energy at 298.15 K)
G4  HT =  -307.223022  (Enthalpy at 298.15 K)
G4  GT =  -307.257859  (Gibbs free energy at 298.15 K)
```

Species 5: benzene

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.000000    1.206843    0.696770
C    -0.000000    0.000000    1.393539
C    -0.000000   -1.206843    0.696770
C    -0.000000   -1.206843   -0.696770
C     0.000000    0.000000   -1.393539
C     0.000000    1.206843   -0.696770
H     0.000000    0.000000   -2.478699
H    -0.000000   -2.146618    1.239352
H    -0.000000   -0.000000    2.478699
H     0.000000   -2.146618   -1.239352
H     0.000000    2.146618    1.239352
H     0.000000    2.146618   -1.239352

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    412.6837    412.6965    616.8121    616.8305    699.6459    722.2103    872.0520
    872.1792    960.5059    960.6148   1008.6967   1014.5758   1016.3494   1061.7862
   1061.8144   1173.5994   1198.0351   1198.0629   1338.5753   1362.0895   1511.4832
   1511.4941   1634.3631   1634.3704   3163.2958   3172.9944   3173.0556   3189.1759
   3189.2419   3200.0498

== Thermochemistry energies (hartree) ==
  ZPVE =     0.098685  (after scaling by 0.9854)
G4  Ee =  -232.192697  (total electronic energy)
G4  U0 =  -232.094012  (Zero-kelvin internal energy)
G4  UT =  -232.089556  (Internal energy at 298.15 K)
G4  HT =  -232.088612  (Enthalpy at 298.15 K)
G4  GT =  -232.120188  (Gibbs free energy at 298.15 K)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.044127   -0.164733    0.263335
C     1.458058    1.153044    0.236331
C     0.204894    1.358210   -0.213721
C    -0.668353    0.243502   -0.744896
C    -0.092645   -1.153534   -0.379659
C     1.301014   -1.265195   -0.067629
H    -0.529696   -1.977484   -0.945474
H    -0.825588   -1.081421    0.688370
H    -0.235555    2.350637   -0.226729
H     2.057616    1.992812    0.574393
O    -1.930778    0.243279   -0.231674
H    -0.798005    0.373994   -1.831859
O    -1.818353   -0.263747    1.066711
H     1.756753   -2.250702   -0.050261
H     3.084952   -0.271852    0.548694

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2081.4514     65.4400    189.9834    340.6806    394.9551    483.0895    501.6953
    583.5703    648.3990    664.9857    748.8786    792.9358    827.8749    905.8037
    932.3641    967.3392    978.2692    985.6127   1001.9949   1030.1643   1098.7304
   1166.8467   1170.6288   1197.0845   1240.8331   1274.1935   1347.2653   1365.4533
   1415.4699   1468.2634   1510.0597   1648.3481   1747.5389   2970.3894   3115.2509
   3165.5329   3172.6995   3185.5274   3198.2842

== Thermochemistry energies (hartree) ==
  ZPVE =     0.111128  (after scaling by 0.9854)
G4  Ee =  -382.993723  (total electronic energy)
G4  U0 =  -382.882595  (Zero-kelvin internal energy)
G4  UT =  -382.876042  (Internal energy at 298.15 K)
G4  HT =  -382.875098  (Enthalpy at 298.15 K)
G4  GT =  -382.914280  (Gibbs free energy at 298.15 K)
```

Species 7: Transition state along ROO· $\xrightarrow{\text{TS2}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.930099   -0.485886   -0.571184
C    -1.700419    0.919147   -0.443245
C    -0.657213    1.401805    0.315314
C     0.247556    0.521682    0.928746
C     0.085658   -0.936519    0.791555
C    -1.115458   -1.375057    0.047418
H     0.232364   -1.482848    1.731975
H     1.012673   -1.258162    0.187623
H    -0.529348    2.471085    0.446250
H    -2.384505    1.611082   -0.923339
O     2.048461    0.639737   -0.402771
H     0.935083    0.897008    1.675350
O     2.356689   -0.544467   -0.642182
H    -1.303660   -2.441692   -0.024272
H    -2.783952   -0.829673   -1.145589

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -164.0472     83.9462    108.5069    132.9001    262.0462    377.1763    448.3527
    572.9756    588.7342    599.0074    704.9926    818.4272    849.5874    899.6663
    925.0614    972.7726    998.5488    999.0399   1002.0455   1015.4883   1130.0275
   1170.8722   1182.2837   1204.0808   1352.7698   1371.2133   1377.7966   1421.6039
   1450.3222   1477.0656   1535.4057   1641.2849   2331.2397   3034.8405   3169.9318
   3177.6204   3188.7684   3198.1340   3214.5468

== Thermochemistry energies (hartree) ==
  ZPVE =     0.112221  (after scaling by 0.9854)
G4  Ee =  -383.010677  (total electronic energy)
G4  U0 =  -382.898456  (Zero-kelvin internal energy)
G4  UT =  -382.891154  (Internal energy at 298.15 K)
G4  HT =  -382.890210  (Enthalpy at 298.15 K)
G4  GT =  -382.931312  (Gibbs free energy at 298.15 K)
```

Species 8: Transition state along ·QOOH$\xrightarrow{\text{TS3}}$ alkene+ ·OOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.129939    0.322467   -0.434348
C     1.759400   -1.012704   -0.191146
C     0.553344   -1.308738    0.399090
C    -0.394513   -0.263674    0.696985
C     0.064060    1.094036    0.544284
C     1.277194    1.367814   -0.048648
H    -0.591944    1.899310    0.858113
H     0.268846   -2.336030    0.596373
H     2.443986   -1.812767   -0.453941
O    -1.611603   -0.471336   -0.606990
H    -1.120899   -0.457661    1.479843
O    -2.796605    0.165476   -0.206867
H    -2.740490    1.018716   -0.662867
H     3.084642    0.543414   -0.898849
H     1.584986    2.396692   -0.205127

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -570.8798     60.9834    118.7750    176.3732    322.4477    382.8403    408.0593
    423.1762    597.9029    601.8888    654.9258    721.1801    812.1019    874.7160
    926.0583    960.6706    963.2890    982.5005   1008.0165   1023.4480   1049.2184
   1105.6918   1165.5993   1169.9099   1195.7653   1327.3685   1358.8438   1386.0986
   1469.9416   1478.5650   1551.9095   1593.7741   3158.8717   3170.4527   3175.5778
   3187.9407   3196.0584   3203.2885   3711.7269

== Thermochemistry energies (hartree) ==
  ZPVE =     0.113763  (after scaling by 0.9854)
G4  Ee =  -383.037315  (total electronic energy)
G4  U0 =  -382.923552  (Zero-kelvin internal energy)
G4  UT =  -382.916130  (Internal energy at 298.15 K)
G4  HT =  -382.915186  (Enthalpy at 298.15 K)
G4  GT =  -382.956419  (Gibbs free energy at 298.15 K)
```

Species 9: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.949345    0.300275   -0.541836
C     1.600493   -1.003920   -0.272913
C     0.431860   -1.291195    0.453988
C    -0.509301   -0.196182    0.829590
C     0.030145    1.186712    0.652810
C     1.165266    1.398934   -0.049862
H    -0.530799    2.008039    1.083679
H     0.178305   -2.300113    0.747496
H     2.235937   -1.819777   -0.600232
O    -1.159327   -0.724067   -0.299595
H    -1.082698   -0.330692    1.752391
O    -2.685663    0.306116   -0.531518
H    -2.428450    0.498365   -1.445059
H     2.853583    0.511573   -1.103052
H     1.527190    2.408464   -0.216973

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -717.7232     74.8417    134.4961    182.6777    213.2320    298.9961    357.7806
    451.4641    568.6267    583.2618    621.4947    734.6745    779.3750    822.8349
    857.5116    905.1142    941.3920    956.6323    981.8317    986.5930    997.0234
   1052.9944   1143.0826   1178.1178   1188.1396   1271.9636   1334.7275   1361.9951
   1424.0060   1466.5478   1514.5586   1638.9198   3051.4699   3171.6929   3181.4588
   3196.1240   3204.6375   3233.8083   3779.6801

== Thermochemistry energies (hartree) ==
  ZPVE =     0.111895  (after scaling by 0.9854)
G4  Ee =  -383.012994  (total electronic energy)
G4  U0 =  -382.901099  (Zero-kelvin internal energy)
G4  UT =  -382.893350  (Internal energy at 298.15 K)
G4  HT =  -382.892406  (Enthalpy at 298.15 K)
G4  GT =  -382.933996  (Gibbs free energy at 298.15 K)
```

Hydrocarbon 10: 2-(cyclohexa-2,4-dien-1-yl)ethyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.011664   -1.110425    0.277232
C    -1.478108   -1.327419   -0.008438
C    -2.312519   -0.284069   -0.099429
C    -1.806555    1.082473    0.040132
C    -0.492938    1.335074   -0.021593
C     0.503334    0.227346   -0.286277
H     0.592235   -1.934351   -0.115081
H     0.138303   -1.123282    1.370972
H    -1.849190   -2.346169   -0.069766
H    -3.377024   -0.431552   -0.254210
H    -2.520079    1.889712    0.176951
H    -0.116504    2.352174    0.054403
C     1.912297    0.570762    0.237509
H     0.583486    0.122395   -1.383618
C     2.968121   -0.392579   -0.178949
H     2.947529   -0.834694   -1.170094
H     3.859336   -0.542552    0.418762
H     1.883682    0.655430    1.332619
H     2.166413    1.585911   -0.122061

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     92.7428    127.7390    145.9200    206.0138    285.3615    370.8510    405.7364
    463.1924    505.5866    542.1560    581.8264    698.2050    768.7338    785.2291
    818.0229    910.6072    936.2716    961.5520    977.1366    986.7605    992.8408
   1038.3794   1090.1033   1094.5560   1116.2382   1174.6969   1184.1106   1204.4708
   1244.9121   1288.9227   1324.5349   1363.0994   1368.6668   1394.7165   1437.4797
   1459.9018   1465.0308   1470.0238   1644.6022   1707.1752   2916.5581   2933.5882
   2960.6803   3025.1265   3071.5026   3143.6534   3149.2059   3160.3792   3174.2574
   3186.8167   3247.6415

== Thermochemistry energies (hartree) ==
  ZPVE =     0.160743  (after scaling by 0.9854)
G4  Ee =  -311.313403  (total electronic energy)
G4  U0 =  -311.152660  (Zero-kelvin internal energy)
G4  UT =  -311.144311  (Internal energy at 298.15 K)
G4  HT =  -311.143367  (Enthalpy at 298.15 K)
G4  GT =  -311.185854  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -310.893403  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.609257   -0.824475    0.749263
C    -1.957790   -1.376051    0.352663
C    -2.891486   -0.586267   -0.190526
C    -2.611346    0.827714   -0.442835
C    -1.360165    1.299064   -0.387372
C    -0.185177    0.383628   -0.111166
H     0.154063   -1.604260    0.678554
H    -0.652844   -0.527833    1.812416
H    -2.169297   -2.417182    0.576976
H    -3.876044   -0.973043   -0.434571
H    -3.438257    1.485320   -0.693697
H    -1.149965    2.344014   -0.601320
C     0.984259    1.172452    0.505357
H     0.155500   -0.005196   -1.084453
C     2.275030    0.392287    0.732555
H     2.138878   -0.495525    1.352713
H     3.043330    1.035369    1.171831
H     0.678901    1.575681    1.480511
H     1.212651    2.037514   -0.129438
O     2.860576   -0.050076   -0.525633
O     2.394258   -1.223045   -0.896512

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     55.7402     71.2979     88.2878    137.1121    188.5633    271.8733    313.6895
    410.5818    424.3850    486.1849    537.5208    544.9939    581.6208    698.3974
    755.1117    786.9743    818.9749    868.7889    920.3942    961.2427    973.1242
    978.0465    992.3505    997.0552   1025.2756   1055.3392   1104.2355   1131.1395
   1182.2696   1184.0899   1202.8280   1218.7940   1244.1566   1281.9088   1325.0545
   1332.7397   1367.8453   1382.6558   1386.2183   1398.0866   1440.2407   1468.2041
   1474.1385   1478.9738   1650.6386   1711.5456   2948.1398   2974.6824   3019.0543
   3058.6548   3068.2796   3082.3704   3133.3060   3149.9784   3162.5183   3176.0070
   3188.8241

== Thermochemistry energies (hartree) ==
  ZPVE =     0.172567  (after scaling by 0.9854)
G4  Ee =  -461.657025  (total electronic energy)
G4  U0 =  -461.484458  (Zero-kelvin internal energy)
G4  UT =  -461.474705  (Internal energy at 298.15 K)
G4  HT =  -461.473761  (Enthalpy at 298.15 K)
G4  GT =  -461.520936  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.131377  (total electronic energy)
```

Species 3: *syn*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.777981    1.305485   -0.167774
C     2.151175    0.993438   -0.685833
C     2.775777   -0.187306   -0.420567
C     2.155069   -1.181575    0.372949
C     0.864747   -0.947788    0.906517
C     0.173097    0.212163    0.678657
H     0.105847    1.532282   -1.014655
H     0.793202    2.251698    0.406249
H     2.636853    1.749375   -1.294917
H     3.768103   -0.373470   -0.820403
H     2.665346   -2.114319    0.581549
H     0.410344   -1.713026    1.531514
C    -1.185126    0.455508    1.278255
H    -0.879892   -1.151429   -1.120507
C    -2.351921    0.555696    0.276240
H    -2.224249    1.391236   -0.421387
H    -3.288282    0.707255    0.826669
H    -1.175346    1.399587    1.845798
H    -1.419464   -0.342692    1.991014
O    -2.574967   -0.639748   -0.455280
O    -1.619690   -0.681529   -1.537418

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     55.8844     70.5048    116.4019    148.5324    208.9811    276.3272    351.1578
    358.5839    399.6448    450.2734    498.6349    535.5809    564.8079    585.7858
    678.7676    733.5142    765.1269    841.8715    887.9998    922.9112    938.9246
    948.1627    972.3203    974.1593    978.5481   1006.0663   1051.3717   1064.7582
   1133.8357   1177.5945   1183.3396   1196.3331   1228.1431   1279.8240   1308.3559
   1339.0058   1368.1022   1391.2112   1407.0337   1421.9042   1430.4637   1441.6973
   1463.0134   1468.4791   1542.7049   1611.6608   2912.4760   2938.6552   2985.2121
   3031.2776   3063.9164   3085.1174   3152.3889   3163.8173   3182.5535   3203.2081
   3708.9467

== Thermochemistry energies (hartree) ==
  ZPVE =     0.171075  (after scaling by 0.9854)
G4  Ee =  -461.674724  (total electronic energy)
G4  U0 =  -461.503649  (Zero-kelvin internal energy)
G4  UT =  -461.493704  (Internal energy at 298.15 K)
G4  HT =  -461.492760  (Enthalpy at 298.15 K)
G4  GT =  -461.539874  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 4: *anti*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.137741    1.288430   -0.247131
C     2.434519    0.824739   -0.842220
C     2.932723   -0.419984   -0.605417
C     2.241502   -1.341958    0.217168
C     1.010428   -0.971146    0.804800
C     0.447037    0.258735    0.611312
H     0.459845    1.632670   -1.051372
H     1.300694    2.210842    0.344681
H     2.973048    1.524899   -1.473350
H     3.877199   -0.715505   -1.052981
H     2.651894   -2.328486    0.397253
H     0.491432   -1.690618    1.432731
C    -0.862075    0.647037    1.243414
H    -3.018302   -0.804843   -1.871170
C    -2.049351    0.703214    0.272066
H    -1.831799    1.340948   -0.596510
H    -2.938867    1.103117    0.775706
H    -0.781251    1.644500    1.698744
H    -1.116479   -0.052745    2.046429
O    -2.290335   -0.630568   -0.147295
O    -3.437485   -0.594330   -1.024469

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     25.8852     55.1364     95.8126    125.7243    204.7119    226.1828    253.9153
    319.5407    354.0321    432.3567    496.1492    533.1866    567.2736    586.5369
    679.5363    740.1891    762.4241    830.0020    918.6352    923.4036    946.7878
    965.0467    971.4205    978.5227    986.6915   1006.0488   1069.4923   1071.5970
   1134.8479   1175.8458   1181.5065   1190.8705   1226.6955   1256.4365   1306.3857
   1341.5869   1362.1221   1382.9088   1395.0875   1422.0328   1430.4523   1441.8013
   1466.2375   1522.1650   1546.6556   1616.0261   2894.2104   2912.6327   2998.0475
   3007.9899   3043.3473   3077.3563   3158.7388   3161.5583   3180.1294   3201.6828
   3750.4943

== Thermochemistry energies (hartree) ==
  ZPVE =     0.170416  (after scaling by 0.9854)
G4  Ee =  -461.672419  (total electronic energy)
G4  U0 =  -461.502003  (Zero-kelvin internal energy)
G4  UT =  -461.491593  (Internal energy at 298.15 K)
G4  HT =  -461.490648  (Enthalpy at 298.15 K)
G4  GT =  -461.539854  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 5: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.397756   -1.256589    0.375285
C    -1.815498   -1.145524   -0.109710
C    -2.407370    0.048707   -0.232140
C    -1.667053    1.274764    0.050035
C    -0.345302    1.264768    0.273711
C     0.458423    0.001069    0.180174
H     0.119630   -2.097948   -0.098857
H    -0.421978   -1.482433    1.454398
H    -2.358904   -2.064532   -0.306963
H    -3.445005    0.129629   -0.539488
H    -2.211728    2.214737    0.052364
H     0.201755    2.188770    0.437706
C     1.811460   -0.007441    0.941002
C     2.461712    0.026494   -0.452382
H     3.090631   -0.833485   -0.713349
H     3.010186    0.945704   -0.693894
H     1.994562   -0.916472    1.517833
H     1.992006    0.861152    1.576903
O     1.179643   -0.022826   -1.105314

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     71.1117     92.9159    222.7642    277.4595    368.8867    397.1420    420.1275
    547.5357    576.9472    668.6623    707.0112    779.5892    804.4161    831.6198
    853.1644    926.5683    950.0229    965.6860    978.6433    984.7370    998.4855
   1009.7974   1025.2501   1037.1214   1145.5303   1156.3840   1169.7697   1203.8154
   1214.1062   1227.7666   1266.1120   1297.5198   1344.0671   1353.1193   1400.9591
   1435.4115   1446.0837   1489.4119   1533.3085   1639.6201   1711.2671   2975.9642
   3011.7007   3047.7053   3063.8367   3071.0750   3125.9231   3154.6511   3165.8993
   3176.3928   3190.8175

== Thermochemistry energies (hartree) ==
  ZPVE =     0.158297  (after scaling by 0.9854)
G4  Ee =  -385.945745  (total electronic energy)
G4  U0 =  -385.787448  (Zero-kelvin internal energy)
G4  UT =  -385.779627  (Internal energy at 298.15 K)
G4  HT =  -385.778682  (Enthalpy at 298.15 K)
G4  GT =  -385.820057  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.477755  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.711343   -1.035674    0.750300
C    -2.075450   -1.252594    0.155934
C    -2.793667   -0.237053   -0.353049
C    -2.259695    1.110140   -0.382481
C    -0.969054    1.352365   -0.042228
C    -0.049915    0.274053    0.307989
H    -0.051826   -1.877173    0.504900
H    -0.802450   -1.052714    1.852515
H    -2.490681   -2.254715    0.204340
H    -3.793387   -0.408865   -0.739215
H    -2.902952    1.924671   -0.698455
H    -0.568667    2.360764   -0.105318
C     1.214278    0.653678    1.080342
H     0.505683   -0.055853   -0.780562
C     2.453278   -0.119901    0.590925
H     2.376841   -1.191426    0.811240
H     3.370476    0.280474    1.033555
H     1.084912    0.465222    2.154767
H     1.412448    1.723830    0.958716
O     2.588873    0.064540   -0.812054
O     1.537254   -0.612577   -1.418305

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1557.2705     79.6945    100.5731    148.8800    224.9850    302.7757    346.2857
    392.2059    424.0598    497.3710    523.3313    549.2753    579.9892    631.8042
    707.5143    759.8903    805.1005    858.0722    918.0009    927.1916    962.9049
    971.8341    977.7069    991.9739    993.5448   1020.0033   1046.1357   1057.7835
   1139.7887   1164.2369   1194.0333   1199.0325   1211.3215   1249.8793   1260.0985
   1320.1310   1353.1068   1359.5693   1377.9516   1407.6207   1450.0129   1462.7877
   1465.2010   1474.0410   1520.6878   1572.7471   1676.1182   2928.5860   3015.0090
   3030.8309   3039.6972   3073.3483   3100.6904   3158.6788   3165.9284   3182.5897
   3194.2898

== Thermochemistry energies (hartree) ==
  ZPVE =     0.167351  (after scaling by 0.9854)
G4  Ee =  -461.626173  (total electronic energy)
G4  U0 =  -461.458822  (Zero-kelvin internal energy)
G4  UT =  -461.449948  (Internal energy at 298.15 K)
G4  HT =  -461.449004  (Enthalpy at 298.15 K)
G4  GT =  -461.493441  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.102187  (total electronic energy)
```

Species 7: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.751152   -0.133259    1.324374
C     1.950392    0.730727    1.079876
C     2.574683    0.749277   -0.113947
C     2.084270   -0.045890   -1.208964
C     0.926420   -0.771424   -1.096482
C     0.146649   -0.740655    0.085256
H    -0.019448    0.420254    1.874682
H     1.043669   -0.957043    2.005051
H     2.324932    1.313981    1.915093
H     3.459641    1.358701   -0.265093
H     2.636950   -0.053368   -2.142634
H     0.556509   -1.341641   -1.942894
C    -1.046022   -1.670749    0.263934
H    -2.253836    2.158769   -1.092113
C    -2.152723   -0.616640    0.174299
H    -2.586935   -0.357756    1.147815
H    -2.971282   -0.860099   -0.511330
H    -1.016665   -2.220187    1.210911
H    -1.094700   -2.397060   -0.551357
O    -1.351657    0.457222   -0.322981
O    -2.584314    1.783669   -0.264295

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -742.1511     69.9140     83.0700     87.3003    159.9739    171.7284    224.4365
    267.7812    302.7345    328.1931    386.0541    454.5238    539.0822    588.4296
    636.9772    712.6765    762.2611    819.6963    834.9399    892.8861    913.4471
    940.2107    960.1079    983.8261    988.7509    992.3932   1001.4077   1051.1970
   1064.0201   1160.3884   1185.4595   1187.3328   1194.2974   1200.6950   1219.9378
   1296.5075   1331.8437   1339.5367   1362.9748   1414.6790   1419.7785   1469.2885
   1487.6904   1501.7921   1529.4322   1657.6348   2914.7441   3018.8485   3041.4979
   3044.0465   3062.1204   3100.6556   3167.7854   3173.1021   3186.6868   3197.4801
   3790.6901   -742.1510     69.9140     83.0695     87.3001    159.9739    171.7290
    224.4364    267.7813    302.7346    328.1931    386.0541    454.5239    539.0822
    588.4295    636.9772    712.6765    762.2612    819.6963    834.9399    892.8861
    913.4471    940.2107    960.1075    983.8261    988.7510    992.3934   1001.4077
   1051.1970   1064.0199   1160.3883   1185.4596   1187.3330   1194.2975   1200.6949
   1219.9378   1296.5074   1331.8438   1339.5367   1362.9750   1414.6790   1419.7787
   1469.2884   1487.6902   1501.7921   1529.4325   1657.6349   2914.7441   3018.8485
   3041.4979   3044.0465   3062.1203   3100.6556   3167.7854   3173.1021   3186.6868
   3197.4801   3790.6902

== Thermochemistry energies (hartree) ==
  ZPVE =     0.168087  (after scaling by 0.9854)
G4  Ee =  -461.622168  (total electronic energy)
G4  U0 =  -461.454081  (Zero-kelvin internal energy)
G4  UT =  -461.443779  (Internal energy at 298.15 K)
G4  HT =  -461.442835  (Enthalpy at 298.15 K)
G4  GT =  -461.490658  (Gibbs free energy at 298.15 K)
```

```
[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.103871  (total electronic energy)
```

Hydrocarbon 11: 6-methyl cyclohepta-2,4-dien-1-yl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.512415    1.302529    0.040143
C     1.135405   -0.018096   -0.332375
C    -0.817001    1.591006    0.153299
C     0.491915   -1.227737    0.387936
C     2.650745    0.010448   -0.077071
H     0.981278   -0.171025   -1.412287
C    -1.930491    0.735367   -0.023962
C    -0.918541   -1.554277   -0.009566
C    -1.946735   -0.671981   -0.173547
H    -1.145530   -2.609745   -0.135551
H     0.538845   -1.047407    1.473218
H     1.119243   -2.108573    0.207387
H    -2.901146    1.223774   -0.043740
H    -2.919309   -1.101601   -0.405750
H     1.209687    2.123823    0.191154
H    -1.064046    2.629449    0.366191
H     2.865300    0.125519    0.991681
H     3.122359    0.846220   -0.603773
H     3.127045   -0.913989   -0.417675

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     91.8440    153.3643    232.8027    318.1169    344.8298    360.1684    401.0839
    465.4948    560.4165    628.1912    679.3108    702.9897    814.8164    832.5759
    870.0952    905.8087    919.6725    936.8072    974.1530    976.3934   1020.8867
   1060.3150   1092.5492   1146.9605   1172.1164   1209.6121   1252.5518   1269.6478
   1303.1025   1339.5687   1356.3553   1386.3555   1407.1426   1426.7360   1458.3784
   1471.8817   1497.9161   1500.6405   1553.9398   1591.3935   2971.1213   2989.9046
   3028.6295   3047.4735   3096.2932   3104.9922   3129.0563   3134.4263   3150.3475
   3158.8528   3169.5100

== Thermochemistry energies (hartree) ==
  ZPVE =     0.163132  (after scaling by 0.9854)
G4  Ee =  -311.346275  (total electronic energy)
G4  U0 =  -311.183143  (Zero-kelvin internal energy)
G4  UT =  -311.175392  (Internal energy at 298.15 K)
G4  HT =  -311.174448  (Enthalpy at 298.15 K)
G4  GT =  -311.215555  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -310.927196  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.708490    0.877040   -0.263984
C     1.207494   -0.540410   -0.175807
C     0.957070    1.986757   -0.220169
C     0.241194   -0.720980    1.015057
C     2.374138   -1.534549   -0.084857
H     0.637783   -0.758307   -1.089383
C    -0.493086    2.079605   -0.111695
C    -1.180443   -0.206964    0.809299
C    -1.399048    1.167786    0.275583
H    -1.715102   -0.302403    1.763452
H     0.653873   -0.222429    1.900608
H     0.159299   -1.785511    1.263635
H    -0.894681    3.052829   -0.389005
H    -2.446969    1.457091    0.250279
H     2.783217    0.999600   -0.383975
H     1.465158    2.942242   -0.326943
H     2.944435   -1.391910    0.840709
H     3.063968   -1.405753   -0.924876
H     2.013302   -2.567198   -0.101559
O    -1.954464   -1.194958    0.000365
O    -1.690428   -1.138537   -1.283303

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     49.3148     93.1259    123.1098    199.8490    234.3772    288.2655    323.2734
    343.4809    356.4657    411.5305    435.2568    526.1404    594.0429    707.0043
    730.9390    748.9127    813.3359    832.1298    881.5001    906.6213    923.4299
    955.3644    999.2854   1002.5735   1020.1897   1064.2155   1102.4300   1129.9398
   1157.8425   1170.6454   1225.8105   1262.8834   1271.8029   1315.0391   1338.0899
   1354.4466   1366.6228   1378.9628   1409.8959   1433.1626   1457.6199   1471.9373
   1498.8436   1502.1519   1674.2306   1711.8745   3015.9812   3023.1831   3028.5439
   3037.0288   3071.5977   3095.5782   3108.7851   3130.0635   3138.3977   3157.1399
   3164.9632

== Thermochemistry energies (hartree) ==
  ZPVE =     0.172340  (after scaling by 0.9854)
G4  Ee =  -461.657017  (total electronic energy)
G4  U0 =  -461.484677  (Zero-kelvin internal energy)
G4  UT =  -461.474891  (Internal energy at 298.15 K)
G4  HT =  -461.473947  (Enthalpy at 298.15 K)
G4  GT =  -461.520515  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.130782  (total electronic energy)
```

Species 3: *syn*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.110654    1.307637    0.387107
C    -1.418760    0.101076   -0.182917
C     0.097152    2.038044    0.322373
C    -0.508597   -0.626843   -1.143004
C    -2.784877   -0.503160   -0.000826
H    -0.095274   -1.089948    1.626407
C     1.369404    1.635876   -0.149105
C     0.970613   -0.823217   -0.765547
C     1.789573    0.419956   -0.602784
H     1.415980   -1.419838   -1.574189
H    -0.522075   -0.096641   -2.108290
H    -0.921532   -1.622219   -1.341473
H     2.135101    2.407332   -0.091229
H     2.844701    0.305812   -0.834044
H    -1.908644    1.789294    0.950159
H     0.054536    3.040923    0.738503
H    -3.307375   -0.596261   -0.963456
H    -3.411448    0.092672    0.667695
H    -2.722156   -1.522236    0.404748
O     1.128700   -1.745543    0.332947
O     0.873182   -1.077595    1.583727

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     74.9756     90.5431    131.3361    183.7959    223.6529    231.4063    290.7620
    330.2508    336.2170    368.4284    438.7114    442.9195    531.1331    578.7490
    679.1461    719.5723    777.3872    793.5949    865.9100    891.7973    904.8480
    925.8345    934.4088    954.2276    984.3751   1004.9948   1041.1903   1051.1562
   1084.5683   1178.0417   1207.9771   1237.4825   1266.9831   1329.6475   1343.6996
   1370.0752   1385.5558   1404.9603   1412.0104   1425.1098   1448.7668   1461.5441
   1475.3426   1490.5891   1553.4744   1603.1192   2985.6629   3001.5986   3013.1445
   3040.9765   3058.5391   3111.3727   3130.1335   3136.0197   3163.7129   3172.4232
   3717.6483

== Thermochemistry energies (hartree) ==
  ZPVE =     0.170594  (after scaling by 0.9854)
G4  Ee =  -461.665418  (total electronic energy)
G4  U0 =  -461.494824  (Zero-kelvin internal energy)
G4  UT =  -461.484569  (Internal energy at 298.15 K)
G4  HT =  -461.483625  (Enthalpy at 298.15 K)
G4  GT =  -461.530656  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 4: *anti*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.543073    0.946630   -0.547668
C     1.548857   -0.278007    0.063369
C     0.600376    1.993277   -0.442915
C     0.532033   -0.718512    1.090072
C     2.651445   -1.259672   -0.211124
H    -2.594334   -0.404356   -1.389372
C    -0.681666    1.988799    0.156347
C    -0.945109   -0.493157    0.734938
C    -1.384151    0.944168    0.686403
H    -1.561289   -1.020455    1.474361
H     0.720915   -0.200516    2.041026
H     0.667514   -1.786568    1.288632
H    -1.183679    2.954932    0.164299
H    -2.373358    1.150186    1.083863
H     2.395181    1.161427   -1.190156
H     0.891739    2.930408   -0.909902
H     3.167570   -1.550418    0.714408
H     3.394512   -0.860191   -0.905704
H     2.244042   -2.185962   -0.638307
O    -1.106641   -1.169357   -0.525690
O    -2.513106   -1.196848   -0.838020

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     58.1876     78.2458    130.5639    185.7571    229.8267    259.0019    288.1203
    320.4274    350.7253    358.5258    428.8577    491.8206    497.5320    597.7132
    681.8536    709.7280    774.9756    793.8980    836.9256    898.5175    920.4693
    931.4435    940.9904    962.6367    981.7509   1011.9249   1043.4811   1059.3269
   1077.6428   1181.1765   1205.8074   1237.4890   1270.2121   1321.6837   1357.0111
   1379.6094   1384.7966   1392.6647   1407.3605   1430.2127   1446.6071   1461.8009
   1475.1123   1489.5992   1552.6256   1601.6792   3003.8656   3008.9310   3022.2102
   3047.7136   3070.9939   3113.2999   3129.8319   3135.1420   3162.9602   3173.3463
   3733.6210

== Thermochemistry energies (hartree) ==
  ZPVE =     0.170833  (after scaling by 0.9854)
G4  Ee =  -461.669337  (total electronic energy)
G4  U0 =  -461.498504  (Zero-kelvin internal energy)
G4  UT =  -461.488249  (Internal energy at 298.15 K)
G4  HT =  -461.487305  (Enthalpy at 298.15 K)
G4  GT =  -461.534676  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 5: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.254391    1.447390    0.099525
C     0.998670    0.127291    0.034772
C    -1.080147    1.574894    0.046069
C     0.497775   -0.910143    1.075165
C     2.492232    0.315937   -0.128609
C    -2.064848    0.494860   -0.031986
C    -0.409493   -1.394736   -0.079541
C    -1.804102   -0.820814   -0.069517
H    -0.426441   -2.470102   -0.277773
H     0.022598   -0.541885    1.984544
H     1.273356   -1.639748    1.315006
H    -3.104563    0.811409   -0.049308
H    -2.631570   -1.523788   -0.111349
H     0.863178    2.345477    0.167149
H    -1.492592    2.580283    0.076774
H     2.904023    0.859341    0.729216
H     2.706804    0.896142   -1.032676
H     2.994845   -0.650766   -0.209184
O     0.447936   -0.709305   -1.033458

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    186.6690    222.6001    247.3711    269.7890    357.5052    398.5863    404.4224
    467.3151    604.2638    608.5854    661.2110    703.4256    790.3078    818.3028
    850.3837    860.3076    879.5640    935.7217    947.3066    964.8246    986.1890
    995.7775   1000.1947   1051.5341   1097.4551   1130.8993   1195.1352   1223.6774
   1244.6348   1252.7998   1268.9040   1296.2931   1367.9437   1403.5366   1410.9391
   1445.6298   1478.2401   1481.6368   1492.5191   1659.0401   1700.8897   3031.9640
   3062.7139   3078.0764   3099.3418   3123.2860   3142.2498   3142.9397   3151.6999
   3165.9125   3176.3414

== Thermochemistry energies (hartree) ==
  ZPVE =     0.158349  (after scaling by 0.9854)
G4  Ee =  -385.945043  (total electronic energy)
G4  U0 =  -385.786694  (Zero-kelvin internal energy)
G4  UT =  -385.779127  (Internal energy at 298.15 K)
G4  HT =  -385.778183  (Enthalpy at 298.15 K)
G4  GT =  -385.818019  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.476576  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.885447    1.499009   -0.258769
C     1.247302    0.130358    0.077382
C    -0.361729    2.040901   -0.256192
C     0.429475   -0.540012    1.177794
C     2.736055   -0.181286    0.108056
H     0.712175   -0.514346   -0.913792
C    -1.636345    1.409121    0.013483
C    -0.970506   -0.960240    0.699369
C    -1.927962    0.147689    0.389164
H    -1.419289   -1.624273    1.446351
H     0.318216    0.124367    2.043877
H     0.948004   -1.442535    1.514792
H    -2.490855    2.062609   -0.152075
H    -2.976770   -0.126287    0.462539
H     1.696078    2.137142   -0.605924
H    -0.434342    3.083466   -0.554959
H     3.201171    0.196154    1.029015
H     3.255990    0.277020   -0.738381
H     2.913024   -1.260186    0.070351
O    -0.782841   -1.857827   -0.424684
O    -0.233888   -1.165469   -1.488255

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1799.7666    117.1355    182.5540    200.3899    220.8473    263.4234    335.6080
    352.0580    374.6077    446.2885    458.5190    495.2187    574.3015    615.1169
    711.3243    742.0033    782.0428    830.5689    864.2878    894.0936    912.9296
    932.8964    972.8134    979.9059    988.8614   1006.6879   1014.6068   1058.3592
   1089.6635   1142.2873   1187.1598   1210.1235   1238.4083   1280.9870   1297.0676
   1327.4977   1339.2339   1373.7882   1408.5090   1437.3026   1460.9380   1475.8539
   1490.9035   1493.9527   1545.9988   1572.0285   1672.1179   3012.8564   3026.5235
   3054.9258   3081.8803   3085.1049   3112.3099   3133.0317   3139.8386   3162.6844
   3171.0030

== Thermochemistry energies (hartree) ==
  ZPVE =     0.166912  (after scaling by 0.9854)
G4  Ee =  -461.625030  (total electronic energy)
G4  U0 =  -461.458118  (Zero-kelvin internal energy)
G4  UT =  -461.449184  (Internal energy at 298.15 K)
G4  HT =  -461.448240  (Enthalpy at 298.15 K)
G4  GT =  -461.491983  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.100700  (total electronic energy)
```

Species 7: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.032014    1.242808   -0.671060
C     1.299438    0.056788    0.085961
C    -0.119905    1.977776   -0.659875
C     0.617556   -0.154451    1.434743
C     2.576066   -0.681321   -0.175809
H    -1.686145   -1.477811   -1.741012
C    -1.369005    1.667407   -0.004765
C    -0.730693   -0.617074    0.879254
C    -1.681397    0.531794    0.656981
H    -1.215826   -1.420250    1.436799
H     0.586161    0.742882    2.059622
H     1.111817   -0.960345    1.980415
H    -2.144709    2.422659   -0.103941
H    -2.679028    0.431735    1.074579
H     1.814642    1.556215   -1.358485
H    -0.126066    2.878989   -1.268059
H     3.378172   -0.289520    0.467204
H     2.898497   -0.580326   -1.215565
H     2.456101   -1.742153    0.055691
O    -0.182168   -1.136583   -0.344830
O    -1.585090   -2.076472   -0.987648

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -769.1943     79.1032    134.7191    151.8649    174.9322    212.5560    240.6062
    254.2048    318.9178    337.2621    388.7913    416.4727    471.9577    530.7640
    613.3856    669.2552    725.6582    807.7962    830.5067    849.8375    874.1486
    897.4268    944.7867    961.0711    981.0939    989.7974   1009.0278   1013.1968
   1032.0336   1065.2919   1142.3599   1206.5088   1221.5997   1255.5083   1269.2413
   1302.5334   1319.4909   1370.9531   1396.6922   1426.1032   1465.2165   1469.4725
   1490.4705   1492.1476   1529.2794   1652.4365   3005.1776   3053.4677   3088.3493
   3088.7563   3116.6127   3130.4539   3139.4705   3148.8258   3165.2096   3177.8741
   3787.5126   -769.1938     79.1033    134.7194    151.8653    174.9324    212.5572
    240.6063    254.2049    318.9178    337.2621    388.7913    416.4727    471.9578
    530.7639    613.3856    669.2552    725.6582    807.7963    830.5067    849.8375
    874.1486    897.4269    944.7867    961.0713    981.0938    989.7972   1009.0278
   1013.1968   1032.0337   1065.2920   1142.3598   1206.5089   1221.5996   1255.5082
   1269.2412   1302.5334   1319.4909   1370.9530   1396.6922   1426.1029   1465.2166
   1469.4725   1490.4705   1492.1476   1529.2793   1652.4364   3005.1776   3053.4677
   3088.3493   3088.7563   3116.6127   3130.4539   3139.4705   3148.8258   3165.2096
   3177.8741   3787.5127

== Thermochemistry energies (hartree) ==
  ZPVE =     0.168117  (after scaling by 0.9854)
G4  Ee =  -461.619793  (total electronic energy)
G4  U0 =  -461.451676  (Zero-kelvin internal energy)
G4  UT =  -461.441524  (Internal energy at 298.15 K)
G4  HT =  -461.440580  (Enthalpy at 298.15 K)
G4  GT =  -461.487148  (Gibbs free energy at 298.15 K)
```

```
[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.100430  (total electronic energy)
```

Hydrocarbon 12: (cyclohepta-3,5-dien-1-yl)methyl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.875801    0.729747   -0.107002
C     1.876173   -0.729090   -0.178029
C     0.873973   -1.590750    0.044287
C     0.862596    1.586672    0.088124
C    -0.554304   -1.270732    0.387935
C    -0.606499    1.315453    0.240044
H     2.863986    1.173913   -0.209749
H     1.123110    2.642333    0.143755
H     2.846681   -1.160786   -0.413805
H     1.106488   -2.650906   -0.029725
C    -1.151926   -0.019267   -0.300413
H    -1.147999    2.126091   -0.266749
H    -0.886425    1.416156    1.300148
H    -0.665152   -1.166040    1.477354
H    -1.172046   -2.135742    0.119063
C    -2.643498   -0.036100   -0.216241
H    -0.856246   -0.081306   -1.363587
H    -3.213750    0.885612   -0.181992
H    -3.192546   -0.964917   -0.326947

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     28.7242     91.1085    139.0890    319.4834    333.2116    362.7480    386.6746
    403.0089    499.0002    524.4212    616.0944    691.3160    779.2795    841.7136
    846.2413    883.8226    892.4954    908.9078    995.3713    999.8804   1014.3846
   1016.5221   1065.6570   1108.5491   1152.7092   1175.7952   1227.2240   1272.4258
   1283.6847   1296.5870   1340.6698   1351.7492   1400.4143   1422.8784   1459.7025
   1461.6463   1465.9605   1474.4326   1687.4366   1716.4649   2923.8378   2989.7031
   3003.4396   3024.0139   3047.8657   3123.9138   3133.7286   3142.3578   3148.5058
   3161.0255   3245.5452

== Thermochemistry energies (hartree) ==
  ZPVE =     0.161367  (after scaling by 0.9854)
G4  Ee =  -311.309416  (total electronic energy)
G4  U0 =  -311.148049  (Zero-kelvin internal energy)
G4  UT =  -311.139644  (Internal energy at 298.15 K)
G4  HT =  -311.138699  (Enthalpy at 298.15 K)
G4  GT =  -311.182244  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -310.889434  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.667263   -0.521979   -0.227361
C     2.528895    0.912129    0.010342
C     1.413994    1.652808    0.072808
C     1.733610   -1.482396   -0.295458
C    -0.007384    1.175467   -0.047449
C     0.248276   -1.399040   -0.090036
H     3.693852   -0.843255   -0.391681
H     2.084037   -2.486512   -0.527334
H     3.474414    1.440290    0.112139
H     1.533504    2.722940    0.224147
C    -0.301733   -0.169418    0.651512
H    -0.058187   -2.297728    0.464508
H    -0.256239   -1.489823   -1.062932
H    -0.290851    1.104883   -1.106560
H    -0.668246    1.942194    0.370201
C    -1.800638   -0.345470    0.917195
H     0.161663   -0.134887    1.646864
O    -2.562103   -0.466117   -0.319578
H    -2.224552    0.495499    1.469973
H    -2.000727   -1.282857    1.445639
O    -2.980694    0.703198   -0.754707

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     30.1657     50.0080     92.9063    108.4701    227.9616    299.9988    336.4239
    361.4965    381.2015    492.4883    523.8423    566.7288    640.7689    689.1578
    780.4974    839.8420    848.8987    864.0819    900.7833    902.9394    912.4439
    994.2156   1006.4573   1012.4153   1018.0511   1062.8406   1094.0208   1141.7416
   1179.4776   1191.4427   1252.1344   1271.8094   1285.4301   1287.8945   1308.5159
   1353.3397   1366.7286   1377.8499   1415.1571   1422.3435   1461.3166   1463.0643
   1469.8746   1479.4731   1687.5799   1716.8118   3000.0279   3012.0041   3018.2423
   3032.4493   3057.8706   3066.7709   3125.5454   3127.3107   3138.4551   3152.4224
   3164.7577

== Thermochemistry energies (hartree) ==
  ZPVE =     0.173008  (after scaling by 0.9854)
G4  Ee =  -461.653283  (total electronic energy)
G4  U0 =  -461.480275  (Zero-kelvin internal energy)
G4  UT =  -461.470473  (Internal energy at 298.15 K)
G4  HT =  -461.469529  (Enthalpy at 298.15 K)
G4  GT =  -461.517526  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.127390  (total electronic energy)
```

Species 3: *syn*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.696769   -0.408432   -0.235345
C     2.436383    0.980243   -0.157779
C     1.217487    1.634666    0.137801
C     1.799864   -1.435552   -0.250922
C     0.022372    1.108684    0.541887
C     0.303783   -1.323176   -0.256486
H     3.746473   -0.679996   -0.327475
H     2.198948   -2.443153   -0.332202
H     3.290721    1.632036   -0.319047
H     1.261494    2.721399    0.094123
C    -0.323071   -0.341895    0.763028
H    -0.123420   -2.316710   -0.077676
H    -0.039547   -1.039849   -1.261549
H    -1.857866    1.055624   -1.336040
H    -0.763722    1.814464    0.794110
C    -1.847893   -0.558898    0.821540
H     0.044054   -0.625144    1.764101
O    -2.503386   -0.484281   -0.438372
H    -2.319997    0.140551    1.522090
H    -2.063967   -1.582306    1.151065
O    -2.647530    0.907937   -0.793356

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     56.0196     72.5339    136.5875    166.8107    220.0721    283.0328    303.8168
    351.6393    391.4513    419.1430    466.6051    545.6163    602.7872    667.7561
    684.6490    707.8231    821.2156    839.4585    871.6006    887.6158    921.1417
    928.4223    941.4498    975.4831    984.7203   1016.7370   1027.9599   1081.7228
   1136.9867   1169.7578   1200.9142   1244.1727   1267.2512   1271.1639   1288.4316
   1349.2103   1361.5289   1387.7489   1389.9275   1399.0236   1428.1527   1454.4704
   1465.8434   1475.0254   1554.0723   1593.2194   2959.4772   3008.5230   3026.0726
   3052.4749   3078.5299   3132.8405   3137.7983   3159.9871   3167.0343   3173.7023
   3725.2076

== Thermochemistry energies (hartree) ==
  ZPVE =     0.171584  (after scaling by 0.9854)
G4  Ee =  -461.660743  (total electronic energy)
G4  U0 =  -461.489159  (Zero-kelvin internal energy)
G4  UT =  -461.479250  (Internal energy at 298.15 K)
G4  HT =  -461.478306  (Enthalpy at 298.15 K)
G4  GT =  -461.525221  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 4: *anti*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.794539   -0.611914   -0.082283
C     2.704116    0.796888   -0.187527
C     1.547259    1.612605   -0.161076
C     1.787777   -1.534070   -0.088253
C     0.270492    1.271129    0.175568
C     0.316445   -1.261120   -0.204751
H     3.807643   -1.007108   -0.040128
H     2.074163   -2.581575   -0.044018
H     3.646709    1.320573   -0.322823
H     1.713654    2.659307   -0.408064
C    -0.197455   -0.078806    0.654952
H    -0.232963   -2.164999    0.085392
H     0.048378   -1.073077   -1.253361
H    -3.963670   -0.703598   -0.764094
H    -0.487228    2.048156    0.130880
C    -1.723210   -0.109029    0.789570
H     0.185008   -0.235096    1.675838
O    -2.261578    0.057149   -0.514227
H    -2.069879    0.706180    1.437943
H    -2.059531   -1.063023    1.220630
O    -3.696180    0.140371   -0.372696

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     66.0164     74.3254    118.6484    153.2231    186.5413    210.3040    314.7851
    332.2777    375.8766    398.7737    434.3478    542.1514    578.5145    669.5969
    686.4520    700.8542    815.6379    859.2156    872.4285    910.6582    918.2522
    937.9348    970.8069    973.3251    977.1268   1018.9938   1050.3719   1090.9446
   1138.9869   1170.7972   1197.4300   1242.7394   1249.4604   1270.7139   1286.6847
   1336.6419   1355.6188   1384.1767   1388.2179   1396.9137   1427.2558   1459.0145
   1472.8257   1520.2440   1554.7490   1591.7746   2977.8412   2997.9763   3013.4962
   3042.6003   3049.0301   3133.1085   3138.0884   3158.4377   3166.0596   3173.1639
   3750.1315

== Thermochemistry energies (hartree) ==
  ZPVE =     0.171247  (after scaling by 0.9854)
G4  Ee =  -461.661980  (total electronic energy)
G4  U0 =  -461.490733  (Zero-kelvin internal energy)
G4  UT =  -461.480567  (Internal energy at 298.15 K)
G4  HT =  -461.479622  (Enthalpy at 298.15 K)
G4  GT =  -461.527164  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 5: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.264833   -0.048953    0.145088
C     1.645547    1.231727   -0.194128
C     0.348220    1.560584   -0.108942
C     1.672806   -1.247579    0.046126
C    -0.759633    0.763197    0.500161
C     0.258920   -1.432798   -0.431975
H     3.309366   -0.006075    0.446408
H     2.241673   -2.136934    0.303060
H     2.331354    1.998983   -0.550257
H     0.037376    2.554804   -0.424882
C    -0.776628   -0.785234    0.492047
H     0.028059   -2.496959   -0.548992
H     0.151423   -0.968931   -1.423477
H    -0.955920    1.164889    1.509259
C    -2.182383   -0.610036   -0.118152
H    -0.747093   -1.240968    1.484164
O    -1.980791    0.810750   -0.282894
H    -3.015262   -0.829515    0.563244
H    -2.364743   -1.110732   -1.076729

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     77.6135    169.1296    268.7964    297.0359    346.2259    389.4649    417.4599
    554.3108    650.9460    690.3408    767.3989    794.8608    845.0916    852.2199
    880.6813    925.3455    967.9620    987.3340    997.8654   1007.0218   1017.3741
   1036.7746   1059.6683   1087.4942   1141.7884   1164.6953   1203.3390   1231.3724
   1251.3595   1264.5255   1287.1884   1331.4461   1344.9600   1372.6058   1380.5307
   1410.3233   1449.5104   1479.4590   1523.9728   1674.9750   1706.3246   2945.2088
   3001.6637   3006.0903   3051.0550   3065.2569   3085.9470   3126.7213   3142.5603
   3153.9085   3169.7487

== Thermochemistry energies (hartree) ==
  ZPVE =     0.159512  (after scaling by 0.9854)
G4  Ee =  -385.939673  (total electronic energy)
G4  U0 =  -385.780161  (Zero-kelvin internal energy)
G4  UT =  -385.772688  (Internal energy at 298.15 K)
G4  HT =  -385.771744  (Enthalpy at 298.15 K)
G4  GT =  -385.812165  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -385.471793  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.640334   -0.347062   -0.179853
C     2.273397    1.048485   -0.169906
C     1.079465    1.618380    0.152722
C     1.814546   -1.409986   -0.200530
C    -0.167965    1.018229    0.573171
C     0.319006   -1.361364   -0.287664
H     3.710264   -0.542862   -0.191561
H     2.265438   -2.399074   -0.198953
H     3.083181    1.738303   -0.396357
H     1.054134    2.706623    0.135154
C    -0.396851   -0.476171    0.757097
H    -0.075439   -2.379548   -0.202189
H     0.019080   -1.009399   -1.284149
H    -1.103416    1.256636   -0.299490
H    -0.647327    1.603804    1.366268
C    -1.924566   -0.728964    0.661491
H    -0.087427   -0.779250    1.767781
O    -2.372691   -0.346156   -0.630334
H    -2.467687   -0.160217    1.425933
H    -2.159384   -1.794051    0.750447
O    -2.304262    1.044874   -0.708672

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1777.7798     92.5416    112.4239    180.8338    255.0585    308.7429    373.5250
    378.7523    423.3234    460.4827    532.8264    566.6355    618.6219    664.7977
    711.2419    782.9526    864.3216    876.4786    898.1026    902.8342    923.9394
    925.9531    972.5665    994.2839   1005.4336   1035.2894   1043.8233   1057.5013
   1108.9995   1152.0080   1209.4320   1221.8278   1261.6642   1271.5562   1274.9846
   1303.4135   1348.9321   1355.0543   1360.9701   1398.3323   1427.2155   1470.5606
   1474.8564   1480.4632   1563.9631   1582.9806   1674.3442   2999.8378   3022.0793
   3029.6826   3052.9263   3065.7101   3099.5487   3132.6391   3141.6528   3157.2051
   3168.4063

== Thermochemistry energies (hartree) ==
  ZPVE =     0.167862  (after scaling by 0.9854)
G4  Ee =  -461.618381  (total electronic energy)
G4  U0 =  -461.450519  (Zero-kelvin internal energy)
G4  UT =  -461.441847  (Internal energy at 298.15 K)
G4  HT =  -461.440903  (Enthalpy at 298.15 K)
G4  GT =  -461.484697  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.094321  (total electronic energy)
```

Species 7: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.706329   -0.015049   -0.379728
C     2.082689    1.281450   -0.273876
C     0.859954    1.613718    0.246483
C     2.094979   -1.214625   -0.346757
C    -0.108059    0.768226    0.847539
C     0.611444   -1.429303   -0.286604
H     3.783821    0.000667   -0.526713
H     2.714750   -2.102448   -0.442007
H     2.705919    2.116854   -0.585331
H     0.631217    2.676039    0.296299
C    -0.157824   -0.746579    0.859851
H     0.397085   -2.501861   -0.241575
H     0.167704   -1.063277   -1.223294
H    -3.152971    0.766592   -1.629754
H    -0.686913    1.234658    1.640169
C    -1.661150   -0.806321    0.569311
H     0.133649   -1.169818    1.828766
O    -1.726212    0.413264   -0.180861
H    -2.273877   -0.742824    1.479018
H    -1.999641   -1.654677   -0.031625
O    -3.397651    0.303110   -0.816797

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -791.1789     68.9482    110.2074    137.5544    146.9086    212.2328    249.0939
    294.6842    318.2839    381.8510    400.7981    429.6186    550.3089    658.4272
    675.1339    712.8220    788.4377    867.8829    877.8298    887.1214    894.1168
    919.1679    932.4988    968.1165    988.0600   1001.4483   1012.6292   1051.7263
   1054.8860   1122.4725   1166.9594   1182.4252   1229.9159   1241.4543   1268.1032
   1274.2059   1325.5291   1352.8491   1363.8737   1418.0893   1429.2705   1476.0853
   1482.1795   1520.2053   1539.5907   1664.9557   3005.0876   3013.5466   3028.6606
   3073.4676   3088.1572   3136.1575   3144.1490   3154.8060   3163.4655   3170.7481
   3789.2615   -791.1792     68.9482    110.2073    137.5541    146.9077    212.2328
    249.0939    294.6842    318.2838    381.8510    400.7981    429.6186    550.3089
    658.4272    675.1339    712.8220    788.4377    867.8829    877.8298    887.1215
    894.1167    919.1679    932.4988    968.1165    988.0599   1001.4484   1012.6292
   1051.7263   1054.8860   1122.4724   1166.9594   1182.4252   1229.9159   1241.4544
   1268.1032   1274.2059   1325.5290   1352.8490   1363.8737   1418.0893   1429.2705
   1476.0853   1482.1794   1520.2053   1539.5907   1664.9558   3005.0876   3013.5466
   3028.6607   3073.4676   3088.1572   3136.1575   3144.1490   3154.8061   3163.4655
   3170.7481   3789.2613

== Thermochemistry energies (hartree) ==
  ZPVE =     0.169303  (after scaling by 0.9854)
G4  Ee =  -461.607085  (total electronic energy)
G4  U0 =  -461.437782  (Zero-kelvin internal energy)
G4  UT =  -461.427886  (Internal energy at 298.15 K)
G4  HT =  -461.426942  (Enthalpy at 298.15 K)
G4  GT =  -461.473567  (Gibbs free energy at 298.15 K)
```

```
[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -461.087905  (total electronic energy)
```

Hydrocarbon 13: cyclohepta-2,4-dien-1-yl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.042696    1.269091   -0.148830
C     1.653895    0.000456   -0.000002
C     1.043398   -1.268516    0.148844
C    -0.273388    1.604966   -0.013387
C    -0.272496   -1.605114    0.013411
C    -1.401061    0.684312    0.355290
C    -1.400655   -0.685088   -0.355319
H    -2.351880    1.185802    0.141613
H    -1.392714    0.513119    1.442400
H    -1.392344   -0.513884   -1.442427
H     1.728480    2.088021   -0.357691
H    -0.533252    2.653340   -0.135362
H    -0.531789   -2.653625    0.135419
H     2.740736    0.000756   -0.000016
H     1.729636   -2.087062    0.357716
H    -2.351207   -1.187106   -0.141693

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    132.7281    186.7183    367.1961    387.1254    427.9678    544.2563    609.5425
    693.2855    706.1469    786.5981    819.6430    885.3514    917.1846    922.0122
    944.8603    977.9057    982.8147   1023.2068   1079.7937   1167.2458   1179.9185
   1251.7818   1253.2055   1283.9270   1341.9585   1373.5074   1386.5998   1430.7680
   1457.1891   1472.8694   1475.3308   1555.1935   1593.4018   2988.6437   2998.5678
   3049.6644   3056.0971   3130.9155   3135.3242   3156.0548   3161.0792   3170.1810


== Thermochemistry energies (hartree) ==
  ZPVE =     0.135735  (after scaling by 0.9854)
G4  Ee =  -272.036967  (total electronic energy)
G4  U0 =  -271.901232  (Zero-kelvin internal energy)
G4  UT =  -271.894911  (Internal energy at 298.15 K)
G4  HT =  -271.893967  (Enthalpy at 298.15 K)
G4  GT =  -271.931779  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -271.671764  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     2.317828    0.296143   -0.146332
C     1.427771    1.448021   -0.068308
C     0.109147    1.527080    0.176992
C     1.985886   -0.999924   -0.242416
C    -0.850990    0.439119    0.528668
C     0.590335   -1.552867   -0.242459
C    -0.316200   -0.950024    0.843328
H     0.632662   -2.638068   -0.108602
H     0.121964   -1.388252   -1.223776
H     0.219028   -0.904905    1.798405
H     3.375384    0.546542   -0.178004
H     2.794065   -1.721256   -0.335701
H     1.927944    2.398915   -0.244171
H    -0.344965    2.514423    0.146674
H    -1.191619   -1.589903    0.993585
O    -1.791040    0.341130   -0.627572
H    -1.487498    0.769450    1.356825
O    -2.912663   -0.245159   -0.285188

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     57.9898     88.2378    193.7853    223.9278    305.3590    333.2879    390.9519
    473.1443    500.7880    555.2133    647.2763    713.9106    780.6695    798.0159
    856.6297    884.2066    899.5009    920.7043    968.9940   1004.2707   1026.6963
   1040.9794   1072.6629   1129.0362   1196.4241   1201.8009   1241.7040   1272.0770
   1284.7793   1314.3788   1362.3653   1378.6586   1390.0483   1431.3569   1460.9766
   1475.8266   1477.4075   1673.5847   1712.2241   3010.8543   3041.7799   3055.0145
   3074.9693   3090.9117   3132.0457   3146.3680   3161.0358   3169.6131

== Thermochemistry energies (hartree) ==
  ZPVE =     0.145071  (after scaling by 0.9854)
G4  Ee =  -422.350400  (total electronic energy)
G4  U0 =  -422.205329  (Zero-kelvin internal energy)
G4  UT =  -422.197005  (Internal energy at 298.15 K)
G4  HT =  -422.196060  (Enthalpy at 298.15 K)
G4  GT =  -422.239455  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.878114  (total electronic energy)
```

Species 3: *syn*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -2.156306   -0.061840   -0.483917
C    -1.596651   -1.290677   -0.060844
C    -0.343833   -1.562424    0.408176
C    -1.601464    1.237408   -0.411474
C     0.788867   -0.589497    0.569793
C    -0.476065    1.641369    0.243770
C     0.414269    0.799782    1.109970
H    -0.225134    2.697947    0.192191
H     2.466292    0.977600   -1.096128
H    -0.056047    0.649605    2.094068
H    -3.139336   -0.130357   -0.941673
H    -2.168854    2.012129   -0.923158
H    -2.257588   -2.149504   -0.162891
H    -0.100279   -2.597644    0.625373
H     1.345691    1.339846    1.304015
O     1.394680   -0.526874   -0.732014
H     1.527769   -1.022089    1.257751
O     2.659643    0.174091   -0.593285

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     50.7715    108.3919    172.4829    253.3618    264.9418    295.2542    359.2985
    412.2076    489.9113    508.4343    556.2937    650.2132    716.9638    778.3398
    804.1635    840.5795    889.4572    915.1233    918.1203    926.2588    953.2711
    982.8668    989.8004   1031.5633   1108.2067   1177.1526   1221.9555   1253.1981
   1259.0746   1336.1233   1342.6270   1376.6749   1389.2242   1392.3586   1435.6565
   1459.9291   1466.6938   1556.7124   1597.9897   2991.7546   3012.2895   3077.8164
   3134.4342   3138.6491   3157.9566   3169.5101   3178.7800   3759.5742

== Thermochemistry energies (hartree) ==
  ZPVE =     0.143365  (after scaling by 0.9854)
G4  Ee =  -422.355992  (total electronic energy)
G4  U0 =  -422.212627  (Zero-kelvin internal energy)
G4  UT =  -422.203894  (Internal energy at 298.15 K)
G4  HT =  -422.202949  (Enthalpy at 298.15 K)
G4  GT =  -422.246964  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 4: *anti*-·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.780255    1.054181   -0.396931
C     0.736741    1.662370    0.341009
C    -0.402417    1.106634    0.850643
C     1.986687   -0.317331   -0.672247
C    -0.862698   -0.317785    0.689090
C     1.320515   -1.395626   -0.168543
C     0.221952   -1.391909    0.855704
H     1.647524   -2.378211   -0.497208
H    -2.212184    1.012880   -1.239313
H     0.649934   -1.269154    1.861728
H     2.521761    1.734684   -0.806707
H     2.805911   -0.534102   -1.354509
H     0.855609    2.732942    0.500167
H    -1.084000    1.761743    1.384933
H    -0.273018   -2.368408    0.852323
O    -1.409480   -0.572440   -0.617027
H    -1.654433   -0.512488    1.423577
O    -2.583433    0.249554   -0.772640

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     65.3358    121.3593    136.8639    252.6857    284.1509    294.4647    363.8387
    415.5229    486.9140    489.8235    579.9225    666.1295    721.3217    784.5427
    787.5008    834.7067    895.9073    920.3552    928.5761    936.3046    961.2052
    981.5156    985.7884   1038.2251   1092.8266   1175.7087   1234.9287   1255.4086
   1261.3503   1325.9360   1359.7914   1379.8793   1390.6972   1400.0732   1435.5472
   1455.6023   1461.9022   1555.5235   1595.7252   2999.2977   3023.1721   3070.4839
   3131.0812   3140.0836   3162.4283   3169.5177   3174.9995   3737.1293

== Thermochemistry energies (hartree) ==
  ZPVE =     0.143499  (after scaling by 0.9854)
G4  Ee =  -422.356111  (total electronic energy)
G4  U0 =  -422.212612  (Zero-kelvin internal energy)
G4  UT =  -422.203914  (Internal energy at 298.15 K)
G4  HT =  -422.202969  (Enthalpy at 298.15 K)
G4  GT =  -422.246771  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =   (total electronic energy)
```

Species 5: *cy*-ether

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.000434    1.618794   -0.732543
C    -0.000434    1.618794    0.732543
C    -0.000434    0.543178    1.534916
C    -0.000434    0.543178   -1.534916
C    -0.051198   -0.879694    1.032900
C    -0.051198   -0.879694   -1.032900
C     1.043972   -1.241847   -0.000000
H    -0.213746   -1.583825   -1.853665
H     1.967113   -0.662179   -0.000000
H     0.016354    2.600869   -1.198153
H     0.019814    0.687506   -2.611635
H     0.016354    2.600869    1.198153
H     0.019814    0.687506    2.611635
H     1.258687   -2.311176   -0.000000
O    -1.063711   -1.046501   -0.000000
H    -0.213746   -1.583825    1.853665

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
    239.4443    241.0836    339.4879    428.7224    464.1666    600.8683    609.1468
    702.8870    789.9060    801.6697    836.1659    856.3050    893.2081    914.8917
    947.0965    965.9556    988.8864    999.3855   1016.2797   1059.4884   1097.9188
   1126.8692   1213.3538   1242.6039   1242.6087   1254.7886   1302.7779   1355.9585
   1375.0172   1408.4563   1443.9377   1481.0947   1660.3061   1700.8733   3065.2927
   3065.6637   3085.4559   3144.9763   3148.3960   3154.5821   3169.5360   3178.1894


== Thermochemistry energies (hartree) ==
  ZPVE =     0.131582  (after scaling by 0.9854)
G4  Ee =  -346.628462  (total electronic energy)
G4  U0 =  -346.496880  (Zero-kelvin internal energy)
G4  UT =  -346.490848  (Internal energy at 298.15 K)
G4  HT =  -346.489904  (Enthalpy at 298.15 K)
G4  GT =  -346.526589  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -346.213771  (total electronic energy)
```

Species 6: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -1.730260    0.777959   -0.447062
C    -1.890919   -0.631152   -0.143700
C    -0.944022   -1.510806    0.236129
C    -0.702728    1.635422   -0.158350
C     0.498223   -1.120724    0.394160
C     0.521949    1.379792    0.558183
C     0.683037    0.093003    1.340032
H     0.968362    2.257674    1.027886
H     1.410963    1.066365   -0.346017
H    -0.047266    0.009723    2.152326
H    -2.574275    1.217369   -0.973625
H    -0.815064    2.650666   -0.533426
H    -2.899606   -1.012891   -0.284607
H    -1.214598   -2.544989    0.419773
H     1.679914    0.070487    1.785619
O     0.941219   -0.765848   -0.951189
H     1.102176   -1.963994    0.747207
O     2.030995    0.079425   -0.882746

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1931.8921    147.2113    232.9771    263.8448    322.1225    400.0806    453.0794
    466.1199    516.1865    597.6468    633.7694    696.6870    761.9086    784.7653
    797.4457    871.7181    898.4616    920.8123    942.0807    969.0960    987.1202
    995.7602   1003.2110   1043.6869   1079.5207   1116.6350   1181.5894   1230.4023
   1239.3681   1261.4373   1292.8543   1333.1986   1365.2003   1396.6956   1428.8375
   1465.9399   1483.6934   1534.7770   1588.3311   1656.1419   3038.6310   3047.8135
   3100.9029   3112.1934   3138.1594   3149.3172   3164.0788   3188.3296

== Thermochemistry energies (hartree) ==
  ZPVE =     0.139857  (after scaling by 0.9854)
G4  Ee =  -422.309109  (total electronic energy)
G4  U0 =  -422.169252  (Zero-kelvin internal energy)
G4  UT =  -422.162024  (Internal energy at 298.15 K)
G4  HT =  -422.161080  (Enthalpy at 298.15 K)
G4  GT =  -422.201166  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.838741  (total electronic energy)
```

Species 7: Transition state along ·QOOH$\xrightarrow{\text{TS4}}$ cycloether+ ·OH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.805312    0.690380   -0.589546
C     1.013440    1.571000    0.237743
C    -0.147172    1.282000    0.867891
C     1.597720   -0.640200   -0.831175
C    -0.816195   -0.070162    0.871089
C     0.619018   -1.456834   -0.192009
C     0.152654   -1.196381    1.233433
H     0.495700   -2.461234   -0.583903
H    -1.950454    0.886041   -1.638758
H     0.956871   -0.924734    1.922882
H     2.621905    1.166075   -1.126860
H     2.187412   -1.106412   -1.616114
H     1.383870    2.590159    0.315790
H    -0.638188    2.069233    1.432564
H    -0.384695   -2.064275    1.617782
O    -1.065623   -0.576938   -0.456565
H    -1.749051   -0.043631    1.436417
O    -2.468380    0.428182   -0.961479

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
   -817.3588     81.3859    150.0101    206.1836    229.8385    284.1591    299.1852
    338.0047    417.4434    480.2473    532.5622    594.2334    718.7306    781.7556
    795.9857    821.8607    860.9180    893.3850    905.8440    932.5248    955.4480
    970.9057    993.3655   1006.9731   1040.5998   1062.1609   1139.9305   1173.2637
   1227.2468   1241.2086   1263.7162   1292.3824   1369.9771   1384.9999   1422.2114
   1465.4987   1483.7249   1527.3581   1647.8170   3058.9928   3094.8701   3125.5216
   3144.3493   3153.1048   3167.5247   3177.5382   3184.2415   3785.8632   -817.3581
     81.3861    150.0103    206.1846    229.8387    284.1592    299.1852    338.0047
    417.4434    480.2474    532.5621    594.2334    718.7306    781.7556    795.9857
    821.8607    860.9181    893.3850    905.8441    932.5248    955.4480    970.9058
    993.3654   1006.9733   1040.5997   1062.1609   1139.9304   1173.2635   1227.2467
   1241.2087   1263.7162   1292.3822   1369.9770   1384.9998   1422.2114   1465.4987
   1483.7247   1527.3580   1647.8170   3058.9929   3094.8701   3125.5216   3144.3493
   3153.1048   3167.5247   3177.5382   3184.2415   3785.8633

== Thermochemistry energies (hartree) ==
  ZPVE =     0.141171  (after scaling by 0.9854)
G4  Ee =  -422.303350  (total electronic energy)
G4  U0 =  -422.162179  (Zero-kelvin internal energy)
G4  UT =  -422.153717  (Internal energy at 298.15 K)
G4  HT =  -422.152773  (Enthalpy at 298.15 K)
G4  GT =  -422.195710  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.837660  (total electronic energy)
```

Hydrocarbon 14: cyclohepta-3,5-dien-1-yl

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.242846    1.581923    0.060190
C     1.131135    1.166811   -0.211383
C     1.662010   -0.054372   -0.056038
C    -1.365594    0.850307    0.151869
C     0.883441   -1.258164    0.438159
C    -1.577444   -0.628599   -0.073704
C    -0.368926   -1.452562   -0.360000
H    -2.311114   -0.747954   -0.883676
H    -2.103311   -1.013111    0.822484
H    -0.318513   -2.024642   -1.279798
H    -0.360720    2.655014    0.202980
H    -2.283174    1.386650    0.390934
H     1.517352   -2.149620    0.395654
H     0.626308   -1.100086    1.496956
H     1.792546    1.966925   -0.537409
H     2.709973   -0.205238   -0.302681

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     83.2259    173.3971    317.9713    328.2929    386.0391    414.3911    525.0893
    633.8837    706.2276    786.4719    833.0060    865.9941    888.3785    897.8879
    913.1925    993.1610   1012.6961   1032.3932   1040.7217   1144.4590   1181.0954
   1237.4500   1247.8702   1265.5906   1305.3438   1347.4047   1372.7251   1413.2218
   1446.0881   1451.2958   1466.9822   1669.5135   1702.7456   2901.7761   2986.9655
   3016.1954   3067.9149   3118.7163   3135.2767   3146.3721   3164.6792   3186.8296


== Thermochemistry energies (hartree) ==
  ZPVE =     0.134265  (after scaling by 0.9854)
G4  Ee =  -272.005688  (total electronic energy)
G4  U0 =  -271.871423  (Zero-kelvin internal energy)
G4  UT =  -271.864628  (Internal energy at 298.15 K)
G4  HT =  -271.863684  (Enthalpy at 298.15 K)
G4  GT =  -271.902604  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -271.639493  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.689079    1.063771   -0.432989
C     1.938523   -0.359297   -0.631934
C     1.308718   -1.416055   -0.101934
C     0.695167    1.684826    0.217967
C     0.153235   -1.414875    0.862915
C    -0.493420    1.115004    0.937345
C    -0.901314   -0.327495    0.659072
H    -1.370644    1.732468    0.708649
H    -0.347730    1.215869    2.022730
H     2.434197    1.709812   -0.892176
H     0.728614    2.772224    0.239252
H    -0.351054   -2.385726    0.808067
H     0.520380   -1.329649    1.895272
H     2.768744   -0.575796   -1.300367
H     1.665020   -2.403515   -0.383089
O    -1.354000   -0.467111   -0.733278
O    -2.471960    0.185072   -0.945724
H    -1.779776   -0.554651    1.271023

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     36.7061     77.3544    135.2147    259.7143    314.3393    331.5842    382.2453
    457.6518    510.2698    531.7394    657.9832    765.9274    770.9577    790.1159
    879.2396    893.7442    902.3649    910.3816    935.9637   1003.2783   1019.3767
   1034.0270   1072.8308   1103.4764   1213.2006   1233.4693   1256.2208   1258.5720
   1282.5414   1339.8446   1353.8439   1385.6503   1403.7514   1432.8102   1453.0239
   1463.5788   1466.6223   1691.3604   1719.8163   3006.4206   3016.9395   3054.7655
   3060.5547   3069.4992   3131.9695   3143.2275   3157.4882   3169.3269

== Thermochemistry energies (hartree) ==
  ZPVE =     0.144888  (after scaling by 0.9854)
G4  Ee =  -422.348939  (total electronic energy)
G4  U0 =  -422.204051  (Zero-kelvin internal energy)
G4  UT =  -422.195612  (Internal energy at 298.15 K)
G4  HT =  -422.194667  (Enthalpy at 298.15 K)
G4  GT =  -422.238765  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.876559  (total electronic energy)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.780171    1.054270   -0.397003
C     1.986731   -0.317239   -0.672259
C     1.320663   -1.395579   -0.168512
C     0.736676    1.662371    0.341023
C     0.222002   -1.391951    0.855650
C    -0.402396    1.106550    0.850749
C    -0.862601   -0.317850    0.689114
H    -2.212333    1.013198   -1.238636
H    -1.083904    1.761593    1.385219
H     2.521594    1.734836   -0.806827
H     0.855489    2.732945    0.500220
H    -0.272971   -2.368448    0.852096
H     0.649926   -1.269376    1.861723
H     2.805996   -0.533968   -1.354488
H     1.647835   -2.378146   -0.497070
O    -1.409522   -0.572409   -0.617198
O    -2.583567    0.249479   -0.772592
H    -1.654398   -0.512625    1.423512

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     65.5825    121.4266    137.0510    252.3990    283.6866    294.5073    363.8361
    415.5501    486.9120    489.8644    579.9980    666.0708    721.3904    784.4459
    787.5640    834.7492    895.9548    920.4408    928.5571    936.2927    961.1220
    981.4871    985.7805   1037.9294   1092.9302   1175.6905   1234.9368   1255.3916
   1261.3723   1326.0210   1359.8396   1379.8923   1391.0158   1400.0738   1435.5622
   1455.6351   1461.8736   1555.4927   1595.7248   2999.3878   3023.3587   3070.5469
   3131.0482   3140.0269   3162.3982   3169.4618   3174.9650   3736.7877

== Thermochemistry energies (hartree) ==
  ZPVE =     0.143499  (after scaling by 0.9854)
G4  Ee =  -422.356110  (total electronic energy)
G4  U0 =  -422.212611  (Zero-kelvin internal energy)
G4  UT =  -422.203912  (Internal energy at 298.15 K)
G4  HT =  -422.202968  (Enthalpy at 298.15 K)
G4  GT =  -422.246766  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.884728  (total electronic energy)
```

Species 4: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     1.859740    1.170556   -0.181296
C     0.683074    1.689367    0.270229
C    -0.535878    0.957034    0.484546
C     2.254187   -0.219373   -0.357031
C    -0.687754   -0.430197   -0.137713
C     1.608153   -1.365312   -0.053631
C     0.192588   -1.527017    0.438738
H     2.672364    1.878081   -0.329371
H     0.678340    2.742796    0.544296
H    -1.676719    1.247667   -0.134800
H     3.272379   -0.335464   -0.721637
H    -0.487242   -0.343787   -1.213694
H     2.158770   -2.290882   -0.198938
H     0.156459   -1.525458    1.536802
H    -0.190910   -2.503719    0.120546
H    -0.960255    1.039163    1.492662
O    -2.649124    0.482553   -0.522316
O    -2.084356   -0.677396    0.037450

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -2197.7970    120.0196    163.0088    247.0915    303.2991    353.8540    379.2505
    447.8785    481.1673    556.6430    628.0892    662.8909    712.5251    791.0412
    853.4560    865.9284    882.9208    912.9446    942.9691    972.5635    989.6921
   1008.8423   1042.9101   1046.9499   1104.8668   1147.3607   1197.9879   1215.7261
   1254.4394   1271.8126   1316.3378   1330.1959   1390.0093   1411.2665   1430.6227
   1467.4397   1473.0223   1545.5907   1656.8953   1759.0545   3011.9894   3022.3226
   3054.6478   3060.2523   3134.6503   3143.0499   3159.2967   3170.3930

== Thermochemistry energies (hartree) ==
  ZPVE =     0.139398  (after scaling by 0.9854)
G4  Ee =  -422.292698  (total electronic energy)
G4  U0 =  -422.153300  (Zero-kelvin internal energy)
G4  UT =  -422.145681  (Internal energy at 298.15 K)
G4  HT =  -422.144737  (Enthalpy at 298.15 K)
G4  GT =  -422.185964  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.822843  (total electronic energy)
```

Hydrocarbon 15: (cyclohexa-2,4-dien-1-yl)methyl (5-membered path)

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.221774   -1.250254   -0.162115
C     1.268477   -1.145672    0.049582
C     1.873379    0.048597    0.040476
C     1.092788    1.273692   -0.134164
C    -0.240273    1.265607   -0.009737
C    -0.986892   -0.014894    0.362643
H    -0.623667   -2.153053    0.308075
H    -0.417508   -1.359349   -1.242647
H     1.842592   -2.062701    0.142282
H     2.951292    0.129319    0.142142
H     1.619848    2.199527   -0.346171
H    -0.821223    2.177184   -0.109398
C    -2.406907   -0.011735   -0.102340
H    -0.985362   -0.056859    1.466134
H    -2.648709   -0.313760   -1.116325
H    -3.190051    0.447645    0.489835

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     81.4892    116.8429    264.3153    301.4382    414.1619    453.9160    500.9285
    561.1430    576.2088    698.8890    763.8156    786.1618    868.3925    946.9159
    954.5692    970.4708    982.2823    992.3213   1045.3252   1091.9210   1123.5583
   1174.5336   1202.4922   1223.8402   1293.8482   1315.6321   1357.4858   1386.4861
   1432.5650   1459.6120   1469.2368   1640.2393   1703.6535   2940.1946   2966.5219
   3070.9180   3140.8689   3155.7943   3164.0841   3180.0523   3188.4808   3246.8748


== Thermochemistry energies (hartree) ==
  ZPVE =     0.132917  (after scaling by 0.9854)
G4  Ee =  -272.004991  (total electronic energy)
G4  U0 =  -271.872074  (Zero-kelvin internal energy)
G4  UT =  -271.864918  (Internal energy at 298.15 K)
G4  HT =  -271.863974  (Enthalpy at 298.15 K)
G4  GT =  -271.903699  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -271.638615  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.373068   -1.075658    0.425215
C    -1.788718   -1.352611   -0.019293
C    -2.638782   -0.344943   -0.251944
C    -2.197471    1.044028   -0.117575
C    -0.896182    1.347575   -0.033781
C     0.154840    0.262748   -0.125454
H     0.298209   -1.886771    0.129912
H    -0.352934   -1.051683    1.528625
H    -2.116424   -2.385810   -0.078705
H    -3.672135   -0.537186   -0.522699
H    -2.947129    1.829392   -0.110199
H    -0.567654    2.381546    0.029915
C     1.447128    0.695177    0.561422
H     0.410200    0.131126   -1.189850
H     1.338705    0.743412    1.649313
H     1.807132    1.654492    0.178951
O     2.510374   -0.278119    0.356984
O     2.934070   -0.263933   -0.887835

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     67.4363     77.2088    131.0957    195.6364    279.8318    329.6978    414.1105
    475.0175    540.1463    562.0659    588.7929    697.9741    782.8079    786.6807
    866.3340    916.3691    947.1464    961.2615    979.8872    990.2338    996.0458
   1054.0055   1107.6190   1121.3879   1170.4037   1187.2191   1206.2427   1225.4493
   1265.5150   1302.8228   1332.1908   1371.0449   1378.9070   1395.4183   1439.0649
   1471.2797   1476.6684   1645.9128   1708.7927   2957.7980   2977.4550   3054.0170
   3084.3756   3116.4879   3154.4153   3166.3937   3179.5541   3191.8386

== Thermochemistry energies (hartree) ==
  ZPVE =     0.144410  (after scaling by 0.9854)
G4  Ee =  -422.350457  (total electronic energy)
G4  U0 =  -422.206047  (Zero-kelvin internal energy)
G4  UT =  -422.197564  (Internal energy at 298.15 K)
G4  HT =  -422.196619  (Enthalpy at 298.15 K)
G4  GT =  -422.240582  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.878349  (total electronic energy)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.592277   -1.303972    0.111329
C    -2.003481   -1.102740   -0.353179
C    -2.588769    0.127000   -0.374506
C    -1.882676    1.285493    0.032963
C    -0.540881    1.170992    0.464386
C     0.105762   -0.032231    0.519831
H     0.001339   -1.820327   -0.664740
H    -0.571479   -2.024262    0.952494
H    -2.556741   -1.981674   -0.669136
H    -3.616261    0.227439   -0.711521
H    -2.364043    2.255892    0.008986
H    -0.004412    2.067708    0.764153
C     1.539664   -0.144078    0.940733
H     1.777691    0.523416   -1.597683
H     1.686813   -0.968342    1.652498
H     1.903438    0.785800    1.391369
O     2.404079   -0.515947   -0.143219
O     2.535871    0.632393   -1.003751

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     47.7704     80.6876    147.4125    195.9884    240.2082    291.1770    371.7038
    435.9250    470.8247    534.2353    579.9983    610.2082    685.0947    767.6818
    769.7076    871.4220    917.4901    939.9801    950.1271    975.8362    976.3064
    984.6544    994.3452   1050.1141   1132.9834   1172.1953   1180.5888   1191.5203
   1265.0386   1307.4395   1346.6234   1367.3332   1395.3605   1420.0377   1431.3460
   1442.0969   1463.7499   1545.4940   1614.3021   2903.9847   2936.0460   3013.6480
   3074.6464   3158.8155   3163.6677   3182.2702   3203.2422   3726.5386

== Thermochemistry energies (hartree) ==
  ZPVE =     0.142614  (after scaling by 0.9854)
G4  Ee =  -422.366270  (total electronic energy)
G4  U0 =  -422.223656  (Zero-kelvin internal energy)
G4  UT =  -422.214737  (Internal energy at 298.15 K)
G4  HT =  -422.213793  (Enthalpy at 298.15 K)
G4  GT =  -422.258641  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.895338  (total electronic energy)
```

Species 4: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.374366   -1.161990   -0.403217
C     1.795696   -1.276168    0.064178
C     2.556341   -0.185453    0.280847
C     2.009501    1.141760    0.119205
C     0.678617    1.324150   -0.121656
C    -0.241760    0.216576   -0.177179
H    -0.260023   -1.933750    0.047491
H     0.355017   -1.389847   -1.486930
H     2.218066   -2.272105    0.156702
H     3.596892   -0.288347    0.571394
H     2.665933    1.998858    0.225847
H     0.274953    2.330983   -0.193201
C    -1.607976    0.418467   -0.862702
H    -0.904934    0.170194    0.929829
H    -1.660185    0.045506   -1.891630
H    -1.891800    1.478368   -0.826157
O    -2.506827   -0.371913   -0.090106
O    -2.216001   -0.003576    1.223831

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1945.8504     91.7659    121.4972    217.2424    261.7050    351.6334    387.6258
    426.9457    544.8273    566.1265    615.5524    666.8029    721.6626    788.2452
    812.9284    906.0236    936.5334    950.7698    960.5038    976.3568    985.1185
    994.0398   1004.8975   1049.0030   1127.8696   1161.7121   1179.2738   1198.0808
   1209.1660   1242.9510   1304.9723   1341.9837   1352.2431   1413.2673   1445.6027
   1473.8997   1484.2638   1519.9171   1657.6127   1727.2445   2913.9295   3012.9046
   3054.2034   3081.8711   3158.6849   3168.6036   3184.6691   3196.3137

== Thermochemistry energies (hartree) ==
  ZPVE =     0.139070  (after scaling by 0.9854)
G4  Ee =  -422.305519  (total electronic energy)
G4  U0 =  -422.166449  (Zero-kelvin internal energy)
G4  UT =  -422.158653  (Internal energy at 298.15 K)
G4  HT =  -422.157708  (Enthalpy at 298.15 K)
G4  GT =  -422.199627  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.835537  (total electronic energy)
```

Hydrocarbon 16: (cyclohexa-2,4-dien-1-yl)methyl (6-membered path)

Species 1: ·R

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.221774   -1.250254   -0.162115
C     1.268477   -1.145672    0.049582
C     1.873379    0.048597    0.040476
C     1.092788    1.273692   -0.134164
C    -0.240273    1.265607   -0.009737
C    -0.986892   -0.014894    0.362643
H    -0.623667   -2.153053    0.308075
H    -0.417508   -1.359349   -1.242647
H     1.842592   -2.062701    0.142282
H     2.951292    0.129319    0.142142
H     1.619848    2.199527   -0.346171
H    -0.821223    2.177184   -0.109398
C    -2.406907   -0.011735   -0.102340
H    -0.985362   -0.056859    1.466134
H    -2.648709   -0.313760   -1.116325
H    -3.190051    0.447645    0.489835

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     81.4892    116.8429    264.3153    301.4382    414.1619    453.9160    500.9285
    561.1430    576.2088    698.8890    763.8156    786.1618    868.3925    946.9159
    954.5692    970.4708    982.2823    992.3213   1045.3252   1091.9210   1123.5583
   1174.5336   1202.4922   1223.8402   1293.8482   1315.6321   1357.4858   1386.4861
   1432.5650   1459.6120   1469.2368   1640.2393   1703.6535   2940.1946   2966.5219
   3070.9180   3140.8689   3155.7943   3164.0841   3180.0523   3188.4808   3246.8748


== Thermochemistry energies (hartree) ==
  ZPVE =     0.132917  (after scaling by 0.9854)
G4  Ee =  -272.004991  (total electronic energy)
G4  U0 =  -271.872074  (Zero-kelvin internal energy)
G4  UT =  -271.864918  (Internal energy at 298.15 K)
G4  HT =  -271.863974  (Enthalpy at 298.15 K)
G4  GT =  -271.903699  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -271.638615  (total electronic energy)
```

Species 2: ROO·

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C     0.206741    1.026832    0.163137
C     1.640847    1.424161   -0.091752
C     2.615317    0.506028   -0.077596
C     2.298187   -0.904253    0.150897
C     1.037991   -1.347516    0.065478
C    -0.082736   -0.404312   -0.325671
H    -0.486371    1.729306   -0.306424
H     0.010196    1.091419    1.246117
H     1.867929    2.478268   -0.217279
H     3.654500    0.790739   -0.208236
H     3.109170   -1.590925    0.373974
H     0.804972   -2.399686    0.205790
C    -1.427531   -0.936639    0.166856
H    -0.132289   -0.390875   -1.428291
H    -1.534443   -0.861249    1.251759
H    -1.580332   -1.971488   -0.155955
O    -2.535949   -0.209131   -0.430712
O    -2.894830    0.826467    0.297018

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     56.9454     90.5071    115.6902    199.3515    279.6498    334.6093    409.6352
    473.0745    535.3500    555.1519    582.9332    698.3417    781.7062    785.4229
    877.2373    911.5971    952.7188    962.6556    979.9109    990.4848    996.1082
   1050.5711   1101.5408   1117.9643   1176.9698   1184.7729   1206.4613   1227.8498
   1265.9529   1307.2621   1331.9755   1370.5964   1377.7819   1393.9548   1438.0420
   1466.6196   1471.7100   1645.4829   1708.0787   2953.7896   2978.9355   3053.4391
   3091.4710   3122.1591   3153.9062   3166.4357   3179.1426   3191.7696

== Thermochemistry energies (hartree) ==
  ZPVE =     0.144356  (after scaling by 0.9854)
G4  Ee =  -422.349653  (total electronic energy)
G4  U0 =  -422.205297  (Zero-kelvin internal energy)
G4  UT =  -422.196787  (Internal energy at 298.15 K)
G4  HT =  -422.195842  (Enthalpy at 298.15 K)
G4  GT =  -422.239919  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.877554  (total electronic energy)
```

Species 3: ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.292506    1.045645    0.327422
C    -1.540248    1.457914   -0.034945
C    -2.590918    0.537881   -0.265032
C    -2.344301   -0.846037   -0.103363
C    -1.115155   -1.311900    0.256206
C     0.067287   -0.407539    0.478833
H     3.046317    1.153589    0.683049
H     0.498360    1.767859    0.488183
H    -1.736746    2.520330   -0.147699
H    -3.575140    0.889279   -0.550810
H    -3.157033   -1.549601   -0.259832
H    -0.950669   -2.378635    0.381829
C     1.245242   -0.846724   -0.449598
H     0.465627   -0.583414    1.496402
H     1.108178   -0.454335   -1.463622
H     1.271640   -1.941887   -0.499761
O     2.538326   -0.532735    0.029799
O     2.768306    0.882905   -0.202909

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
     33.2486     80.8888    143.7233    188.2660    234.3127    314.4852    366.1236
    405.8116    477.4889    576.4890    590.5180    619.7169    670.7601    748.6361
    790.0309    846.1647    888.5317    939.1272    963.5336    971.8884    985.1885
    995.9981   1027.5310   1049.9152   1062.1172   1121.3707   1171.9471   1201.1485
   1228.8578   1276.4271   1323.1827   1347.7570   1372.2278   1395.1512   1403.4599
   1450.4348   1461.3010   1540.6634   1603.3283   2902.7124   3030.0591   3085.3368
   3153.6247   3163.9021   3173.6687   3201.7353   3209.2677   3769.8459

== Thermochemistry energies (hartree) ==
  ZPVE =     0.142682  (after scaling by 0.9854)
G4  Ee =  -422.359323  (total electronic energy)
G4  U0 =  -422.216641  (Zero-kelvin internal energy)
G4  UT =  -422.207674  (Internal energy at 298.15 K)
G4  HT =  -422.206730  (Enthalpy at 298.15 K)
G4  GT =  -422.251971  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.888321  (total electronic energy)
```

Species 4: Transition state along ROO· $\xrightarrow{\text{TS1}}$ ·QOOH

```
[ G4 data ]

== B3LYP/6-31G(2df,p) equilibrium geometry (Angstrom) ==
C    -0.076380   -0.870836    0.404425
C    -1.349192   -1.458976   -0.002584
C    -2.405218   -0.639401   -0.245868
C    -2.311243    0.800143   -0.033578
C    -1.115208    1.395961    0.115715
C     0.109996    0.542274   -0.114624
H     1.145336   -1.304173    0.005886
H     0.184258   -1.043608    1.457754
H    -1.487287   -2.535928    0.022375
H    -3.376404   -1.063148   -0.482794
H    -3.231126    1.373121    0.024847
H    -1.015225    2.465441    0.272985
C     1.494603    1.065024    0.254113
H     0.156360    0.436191   -1.217504
H     1.697650    1.011690    1.331655
H     1.669183    2.082299   -0.109663
O     2.426651    0.252897   -0.468447
O     2.344988   -1.056274    0.022055

== B3LYP/6-31G(2df,p) harmonic frequencies (cm^-1) ==
  -1983.3502    127.4770    154.9539    268.0826    337.5470    379.3726    414.7620
    425.7750    459.1096    566.8117    589.3298    619.2654    699.3834    774.4366
    817.2972    902.8914    919.4433    952.6876    973.5887    980.0878    994.4194
   1010.9672   1040.8016   1066.6189   1109.0186   1149.7503   1183.4176   1198.9237
   1238.7318   1256.0162   1285.3999   1302.4661   1354.6410   1374.3631   1400.5993
   1436.5201   1476.3237   1530.7054   1574.6996   1654.6619   2896.3514   3020.7440
   3023.8798   3097.9766   3161.8151   3168.8210   3181.6788   3192.8933

== Thermochemistry energies (hartree) ==
  ZPVE =     0.138613  (after scaling by 0.9854)
G4  Ee =  -422.297622  (total electronic energy)
G4  U0 =  -422.159009  (Zero-kelvin internal energy)
G4  UT =  -422.151449  (Internal energy at 298.15 K)
G4  HT =  -422.150505  (Enthalpy at 298.15 K)
G4  GT =  -422.191566  (Gibbs free energy at 298.15 K)

[ CCSDT-F12a/cc-pVDZ-F12 data ]

CCSD(T)-F12a/cc-pVDZ-F12  Ee =  -421.827476  (total electronic energy)
```

References

(1) Martin, J. M.; de Oliveira, G. Towards standard methods for benchmark quality ab initio thermochemistry—W1 and W2 theory. *J. Chem. Phys* . **1999**, *111*, 1843–1856.

(2) Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-4 theory. *J. Chem. Phys* . **2007**, *126*, 084108.