Supporting Information
OH Radical Yields from the Ozone Reaction with Cycloalkenes

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The minima and transition structures reported here were obtained with Gaussian 94 and Gaussian 98, using the (U)B3LYP/6-31G(d,p) method. The quantities which depend on the vibrational frequencies are shown here unscaled. The results reported in the main body of the paper were obtained by scaling by 0.963.

Cis-Butene Primary Ozonide

```
SCF Done:  E(RB+HF-LYP) =  -382.744083324     A.U. after    1 cycles
            Convg  =     .2438D-08             -V/T =  2.0088
            S**2   =    .0000

                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          6            .232118    -.785989     .472588
   2          1            .113363   -1.130335    1.508573
   3          8           -.940660   -1.123299    -.277721
   4          8           -.962200    1.109616    -.269979
   5          6            .219998     .789195     .473834
   6          8          -1.821870    -.016139     .006975
   7          1            .101953    1.130376    1.510935
   8          6           1.408580   -1.487269    -.186889
   9          1           1.252588   -2.569409    -.171874
  10          1           1.525563   -1.172169   -1.226196
  11          1           2.334136   -1.274164     .356381
  12          6           1.381287    1.509931    -.191528
  13          1           1.497633    1.197739   -1.231783
  14          1           1.207496    2.589380    -.174788
  15          1           2.313210    1.311952     .346517
---------------------------------------------------------------------

Zero-point correction=                           .122534 (Hartree/Particle)
Thermal correction to Energy=                    .129742
Thermal correction to Enthalpy=                  .130686
Thermal correction to Gibbs Free Energy=         .090586
Sum of electronic and zero-point Energies=          -382.621550
Sum of electronic and thermal Energies=             -382.614342
Sum of electronic and thermal Enthalpies=           -382.613397
Sum of electronic and thermal Free Energies=        -382.653497

                       E                     CV                    S
                  KCAL/MOL           CAL/MOL-KELVIN       CAL/MOL-KELVIN
TOTAL                81.414                26.246                84.397
```

Cis-Butene Primary Ozonide Syn Cycloreversion Transition Structure

```
CF Done:  E(RB+HF-LYP) =  -382.711736710     A.U. after   19 cycles
             Convg  =    0.9583D-08             -V/T =  2.0089
             S**2   =   0.0000

                   Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          1          -0.947575   -1.033378    1.379189
    2          6          -0.928797   -0.615705    0.353349
    3          8          -0.414664   -1.340083   -0.568385
    4          6           0.409034    0.712350    0.612669
    5          6          -2.186810    0.200061    0.023680
    6          1           0.242744    1.158492    1.593935
    7          8           1.418749   -0.173492    0.705503
    8          6           0.385172    1.619431   -0.588716
    9          1          -2.383695    0.975890    0.770126
   10          1          -2.116600    0.645006   -0.969951
   11          1          -3.036224   -0.490734    0.025339
   12          8           1.617595   -0.774807   -0.458053
   13          1          -0.394227    2.375121   -0.479053
   14          1           0.235385    1.052516   -1.506176
   15          1           1.355160    2.127311   -0.651820
 ---------------------------------------------------------------------

 Zero-point correction=                           0.119499 (Hartree/Particle)
 Thermal correction to Energy=                    0.126891
 Thermal correction to Enthalpy=                  0.127835
 Thermal correction to Gibbs Free Energy=         0.088376
 Sum of electronic and zero-point Energies=           -382.592238
 Sum of electronic and thermal Energies=              -382.584846
 Sum of electronic and thermal Enthalpies=            -382.583902
 Sum of electronic and thermal Free Energies=         -382.623361

                     E (Thermal)             CV                S
                      KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                   79.625             26.762             83.049
```

Cis-Butene Primary Ozonide Anti Cycloreversion Transition Structure

```
 SCF Done:  E(RB+HF-LYP) =  -382.716297541     A.U. after   19 cycles
             Convg  =     .6700D-08             -V/T =  2.0089
             S**2   =    .0000

                   Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic              Coordinates (Angstroms)
 Number     Number             X           Y           Z
 ---------------------------------------------------------------------
    1          6            .802008     .678868     .511274
    2          1            .545678    1.099562    1.504712
    3          8           1.622907    -.298512     .499323
```

4	6	-.878753	-.242168	.412650
5	6	.853358	1.696288	-.623870
6	6	-2.065147	.634625	.142269
7	8	-.533779	-1.034043	-.612426
8	1	-.796932	-.737973	1.378728
9	1	1.804734	2.235361	-.564901
10	1	.817733	1.187722	-1.590386
11	1	.045436	2.432147	-.564360
12	8	.464529	-1.841371	-.269829
13	1	-2.074071	1.477471	.838259
14	1	-2.995122	.073112	.287306
15	1	-2.045504	1.018325	-.879847

Zero-point correction= .119074 (Hartree/Particle)
Thermal correction to Energy= .126626
Thermal correction to Enthalpy= .127570
Thermal correction to Gibbs Free Energy= .087688
Sum of electronic and zero-point Energies= -382.597224
Sum of electronic and thermal Energies= -382.589672
Sum of electronic and thermal Enthalpies= -382.588728
Sum of electronic and thermal Free Energies= -382.628609

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	79.459	27.032	83.939

Trans-Butene Primary Ozonide

SCF Done: E(RB+HF-LYP) = -382.746435157 A.U. after 8 cycles
Convg = .4880D-08 -V/T = 2.0088
S**2 = .0000

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	.758378	-.267508	-.361783
2	1	.635460	-.577031	-1.408813
3	8	.868004	1.158439	-.296672
4	1	-.356020	-1.053218	1.373828
5	8	-1.055995	.737637	.761809
6	6	-.566593	-.566777	.414697
7	8	-.511795	1.565061	-.300667
8	6	2.020338	-.861595	.241578
9	1	2.904221	-.536894	-.313900
10	1	2.128989	-.549216	1.283770
11	1	1.978821	-1.954394	.201556
12	6	-1.578429	-1.360493	-.400016
13	1	-1.165303	-2.334184	-.686912
14	1	-2.490063	-1.532810	.177813
15	1	-1.839977	-.813107	-1.309969

```
Zero-point correction=                           .122444 (Hartree/Particle)
Thermal correction to Energy=                    .129618
Thermal correction to Enthalpy=                  .130562
Thermal correction to Gibbs Free Energy=         .091197
Sum of electronic and zero-point Energies=          -382.623991
Sum of electronic and thermal Energies=             -382.616817
Sum of electronic and thermal Enthalpies=           -382.615873
Sum of electronic and thermal Free Energies=        -382.655238

                       E                     CV                S
                  KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                81.336             26.272             82.850
```

Trans-Butene Primary Ozonide Syn Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -382.716035409     A.U. after    5 cycles
            Convg  =     .6120D-08             -V/T =  2.0089
            S**2   =    .0000

                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -.952062    -.421129     .467886
   2          8             0       -.650978     .585588    1.199564
   3          6             0        .608038    -.612286    -.586329
   4          1             0       -.812038   -1.418537     .930282
   5          6             0      -2.142099    -.319411    -.479652
   6          1             0        .369623   -1.227952   -1.454217
   7          8             0        .637464     .679025    -.971788
   8          6             0       1.673493   -1.102608     .357151
   9          1             0      -2.072853     .592911   -1.076460
  10          1             0      -2.213988   -1.186968   -1.143862
  11          1             0      -3.062175    -.266399     .111893
  12          8             0        .867585    1.473974     .065114
  13          1             0       1.588304   -2.185222     .476968
  14          1             0       1.588212    -.610370    1.325057
  15          1             0       2.658119    -.873550    -.067119
---------------------------------------------------------------------

Zero-point correction=                           .119069 (Hartree/Particle)
Thermal correction to Energy=                    .126587
Thermal correction to Enthalpy=                  .127531
Thermal correction to Gibbs Free Energy=         .087785
Sum of electronic and zero-point Energies=          -382.596966
Sum of electronic and thermal Energies=             -382.589448
Sum of electronic and thermal Enthalpies=           -382.588504
Sum of electronic and thermal Free Energies=        -382.628250

                  E (Thermal)             CV                S
                   KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                79.435             26.925             83.652
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Trans-Butene Primary Ozonide Anti Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -382.715642618     A.U. after    6 cycles
            Convg  =     .7827D-08             -V/T =  2.0089
            S**2   =    .0000

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1             0         .812752     .486127   -1.467818
   2          6             0        1.013344     .028299    -.478963
   3          8             0        1.035706   -1.246146    -.419151
   4          6             0        -.702500     .470424     .314870
   5          6             0        1.989233     .816971     .397689
   6          6             0       -1.277826    1.762675    -.182645
   7          8             0       -1.363018    -.613893    -.096278
   8          1             0        -.348553     .402200    1.342547
   9          1             0        2.055766     .358743    1.387809
  10          1             0        2.982994     .776002    -.060583
  11          1             0        1.711160    1.871791     .495174
  12          8             0        -.807918   -1.721660     .379338
  13          1             0        -.515471    2.545709    -.161466
  14          1             0       -2.107625    2.090389     .453816
  15          1             0       -1.642692    1.652420   -1.206464
---------------------------------------------------------------------

Zero-point correction=                           .118941 (Hartree/Particle)
Thermal correction to Energy=                    .126574
Thermal correction to Enthalpy=                  .127518
Thermal correction to Gibbs Free Energy=         .087292
Sum of electronic and zero-point Energies=          -382.596702
Sum of electronic and thermal Energies=             -382.589069
Sum of electronic and thermal Enthalpies=           -382.588124
Sum of electronic and thermal Free Energies=        -382.628351

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                   79.426            27.135             84.663
```

Cyclopentene Primary Ozonide (best conformer)

```
SCF Done:  E(RB+HF-LYP) =  -420.850979506     A.U. after    8 cycles
            Convg  =     .7812D-08             -V/T =  2.0088
            S**2   =    .0000

                  Standard orientation:
-----------------------------------------------------------
Center     Atomic             Coordinates (Angstroms)
Number     Number            X           Y           Z
-----------------------------------------------------------
   1          1          1.217122    -.000421   -1.674842
   2          6          1.732254     .000201    -.709459
   3          6          1.264073    1.205894     .126024
```

4	6	1.264994	-1.205316	.126731
5	1	2.809111	.000447	-.898917
6	6	-.110568	.784004	.658944
7	6	-.110037	-.783854	.659000
8	1	1.207908	2.143370	-.433886
9	1	1.937154	1.366585	.976847
10	1	1.209643	-2.143242	-.432503
11	1	1.938143	-1.364850	.977716
12	1	-.377558	1.207359	1.633442
13	8	-1.105047	1.117991	-.316828
14	8	-1.103873	-1.118140	-.317414
15	1	-.377561	-1.207293	1.633283
16	8	-2.017112	-.000793	-.234332

Zero-point correction= .131067 (Hartree/Particle)
Thermal correction to Energy= .137469
Thermal correction to Enthalpy= .138413
Thermal correction to Gibbs Free Energy= .100488
Sum of electronic and zero-point Energies= -420.719912
Sum of electronic and thermal Energies= -420.713511
Sum of electronic and thermal Enthalpies= -420.712567
Sum of electronic and thermal Free Energies= -420.750492

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	86.263	25.271	79.820

Cyclopentene Primary Ozonide Anti Transition Structure

SCF Done: E(RB+HF-LYP) = -420.822191485 A.U. after 7 cycles
Convg = .6649D-08 -V/T = 2.0089
S**2 = .0000

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	2.925097	-.108159	-.759447
2	6	2.098406	.032260	-.057765
3	6	1.119521	1.130054	-.494725
4	6	1.259416	-1.266297	.102365
5	1	2.541979	.299195	.909161
6	6	-.082959	1.038811	.455841
7	6	-.135127	-.850917	.504327
8	1	.762208	.972919	-1.517755
9	1	1.571357	2.126977	-.443986
10	1	1.186069	-1.785622	-.858797
11	1	1.698982	-1.957255	.826877
12	1	.194215	1.183055	1.521093
13	8	-1.261586	1.399103	.116583
14	8	-1.042391	-1.017214	-.473797
15	1	-.534157	-.997100	1.505997
16	8	-2.183685	-.411573	-.173211

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Zero-point correction=                           .128090 (Hartree/Particle)
Thermal correction to Energy=                    .134754
Thermal correction to Enthalpy=                  .135698
Thermal correction to Gibbs Free Energy=         .097256
Sum of electronic and zero-point Energies=          -420.694101
Sum of electronic and thermal Energies=             -420.687437
Sum of electronic and thermal Enthalpies=           -420.686493
Sum of electronic and thermal Free Energies=        -420.724936

                       E                     CV                S
                  KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                84.560             25.899             80.909
```

Cyclopentene Primary Ozonide Syn Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -420.823801036     A.U. after    1 cycles
            Convg  =     .4528D-08             -V/T =  2.0089
            S**2   =    .0000

                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1             0        2.474491   -1.069175    -.939891
   2          6             0        1.534001    -.555623    -.720265
   3          6             0        1.705351     .625082     .238229
   4          6             0         .278117    1.073917     .580097
   5          6             0        -.452580    -.681856     .823827
   6          6             0         .517585   -1.486790    -.033695
   7          1             0        1.113144    -.188716   -1.659448
   8          1             0        2.259012    1.456202    -.209389
   9          1             0        2.229766     .321628    1.153819
  10          1             0         .094759    1.479477    1.591191
  11          8             0        -.427706    1.563659    -.374949
  12          8             0       -1.689860    -.422686     .372618
  13          1             0        -.523612    -.928837    1.883093
  14          1             0        -.069663   -2.062161    -.756648
  15          1             0        1.030455   -2.189551     .631421
  16          8             0       -1.645333     .025621    -.875581
---------------------------------------------------------------------

Zero-point correction=                           .128441 (Hartree/Particle)
Thermal correction to Energy=                    .135045
Thermal correction to Enthalpy=                  .135989
Thermal correction to Gibbs Free Energy=         .097678
Sum of electronic and zero-point Energies=          -420.695360
Sum of electronic and thermal Energies=             -420.688756
Sum of electronic and thermal Enthalpies=           -420.687812
Sum of electronic and thermal Free Energies=        -420.726123

                  E (Thermal)             CV                S
```

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	84.742	25.589	80.633

Cyclohexene Primary Ozonide (best conformer)

```
SCF Done:  E(RB+HF-LYP) =  -460.167900806     A.U. after    1 cycles
            Convg  =     .6301D-08             -V/T =  2.0090
            S**2   =    .0000
```

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.170758	-1.322858	.463332
2	6	-1.963606	-.450176	-.516476
3	6	.285599	-.878447	.622974
4	1	-1.188054	-2.376201	.164128
5	1	-1.632748	-1.275842	1.459075
6	6	-1.855714	1.032520	-.137505
7	6	.504413	.643498	.742114
8	1	-3.011229	-.770539	-.524835
9	1	-1.575380	-.597512	-1.531303
10	1	.745364	-1.370743	1.490898
11	8	1.033934	-1.224947	-.547655
12	6	-.390628	1.494927	-.163549
13	1	-2.284954	1.187791	.863019
14	1	-2.444737	1.649599	-.824745
15	1	.463685	.962251	1.788769
16	8	1.887307	.722346	.380285
17	8	1.925754	-.057594	-.820024
18	1	-.301457	2.545599	.132051
19	1	-.002297	1.410383	-1.183248

```
Zero-point correction=                           .160328 (Hartree/Particle)
Thermal correction to Energy=                    .167874
Thermal correction to Enthalpy=                  .168818
Thermal correction to Gibbs Free Energy=         .128286
Sum of electronic and zero-point Energies=          -460.007573
Sum of electronic and thermal Energies=             -460.000027
Sum of electronic and thermal Enthalpies=           -459.999083
Sum of electronic and thermal Free Energies=        -460.039615
```

	E KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	105.342	29.970	85.307

Cyclohexene Primary Ozonide Syn Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -460.140562307     A.U. after    7 cycles
            Convg  =     .4216D-08             -V/T =  2.0091
            S**2   =    .0000
```

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.386474	-1.177210	.492942
2	6	-2.068086	-.194621	-.455814
3	6	.159047	-1.206982	.385533
4	1	-1.713646	-2.203898	.290089
5	1	-1.656694	-.960327	1.534748
6	6	-1.686548	1.249612	-.116484
7	6	.605608	.573531	.774822
8	1	-3.154849	-.320316	-.395114
9	1	-1.770839	-.426879	-1.484348
10	1	.624407	-1.717563	1.252700
11	8	.698224	-1.382571	-.759807
12	6	-.168474	1.453754	-.180933
13	1	-2.061598	1.505608	.884534
14	1	-2.163403	1.946688	-.813760
15	1	.445070	.722534	1.844416
16	8	1.927148	.406572	.556902
17	8	2.178655	.165741	-.722129
18	1	.088702	2.491648	.074274
19	1	.200200	1.256065	-1.187673

Zero-point correction= .157467 (Hartree/Particle)
Thermal correction to Energy= .165149
Thermal correction to Enthalpy= .166093
Thermal correction to Gibbs Free Energy= .125469
Sum of electronic and zero-point Energies= -459.983095
Sum of electronic and thermal Energies= -459.975414
Sum of electronic and thermal Enthalpies= -459.974469
Sum of electronic and thermal Free Energies= -460.015093

	E KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	103.632	30.318	85.499

Cyclohexene Primary Ozonide Anti Cycloreversion Transition Structure

SCF Done: E(RB+HF-LYP) = -460.143273686 A.U. after 6 cycles
Convg = .3583D-08 -V/T = 2.0090
S**2 = .0000

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.008542	-1.402140	.592619
2	6	-1.950671	-.692907	-.394716
3	6	.406169	-.883082	.557547

4	1	-.993859	-2.484918	.410147
5	1	-1.372011	-1.266952	1.618037
6	6	-1.992381	.824048	-.166067
7	6	.462288	1.017735	.595348
8	1	-2.953758	-1.119860	-.287686
9	1	-1.626104	-.901512	-1.421176
10	1	1.062522	-1.057752	1.408899
11	8	1.034707	-1.014787	-.618256
12	6	-.626955	1.493753	-.370349
13	1	-2.357616	1.028749	.851090
14	1	-2.722427	1.275544	-.846820
15	1	.173620	1.042510	1.667823
16	8	1.685439	1.255341	.324376
17	8	2.283430	-.561783	-.538143
18	1	-.719166	2.580029	-.241541
19	1	-.259258	1.329551	-1.388886

Zero-point correction= .157081 (Hartree/Particle)
Thermal correction to Energy= .164818
Thermal correction to Enthalpy= .165763
Thermal correction to Gibbs Free Energy= .125012
Sum of electronic and zero-point Energies= -459.986193
Sum of electronic and thermal Energies= -459.978455
Sum of electronic and thermal Enthalpies= -459.977511
Sum of electronic and thermal Free Energies= -460.018261

	E	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	103.425	30.537	85.766

Cycloheptene Primary Ozonide (best conformer)

SCF Done: E(RB+HF-LYP) = -499.482932868 A.U. after 1 cycles
Convg = 0.1738D-08 -V/T = 2.0090
S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.597072	0.000145	0.218812
2	6	0	2.579406	0.000014	-0.191185
3	6	0	1.885620	-1.305146	0.229163
4	6	0	1.885656	1.305470	0.228287
5	1	0	2.692929	-0.000371	-1.284273
6	6	0	0.480346	-1.515313	-0.363546
7	6	0	0.480098	1.514996	-0.363948
8	1	0	1.834104	-1.363890	1.325813
9	1	0	2.520073	-2.142133	-0.083912
10	1	0	1.834597	1.365162	1.324908
11	1	0	2.519893	2.142246	-0.085791
12	1	0	0.230124	-2.581891	-0.338300

13	6	0	-0.622633	-0.785715	0.397447
14	6	0	-0.622388	0.785417	0.397801
15	1	0	0.229606	2.581520	-0.338983
16	1	0	0.456348	-1.216871	-1.417612
17	1	0	0.455721	1.216177	-1.417900
18	1	0	-0.641980	-1.129364	1.441140
19	1	0	-0.640614	1.128649	1.441654
20	8	0	-1.864596	1.117186	-0.234236
21	8	0	-1.864379	-1.116749	-0.235796
22	8	0	-2.706588	-0.000152	0.121323

Zero-point correction= 0.189444 (Hartree/Particle)
Thermal correction to Energy= 0.198090
Thermal correction to Enthalpy= 0.199034
Thermal correction to Gibbs Free Energy= 0.155655
Sum of electronic and zero-point Energies= -499.293489
Sum of electronic and thermal Energies= -499.284843
Sum of electronic and thermal Enthalpies= -499.283898
Sum of electronic and thermal Free Energies= -499.327278

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	124.304	34.581	91.300

Cycloheptene Primary Ozonide Anti Cycloreversion Transition Structure

SCF Done: E(RB+HF-LYP) = -499.452776376 A.U. after 1 cycles
Convg = 0.8902D-08 -V/T = 2.0091
S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.546545	-0.002623	0.015054
2	6	0	2.492807	-0.058594	-0.285260
3	6	0	1.835342	-1.203505	0.506283
4	6	0	1.882777	1.342087	-0.127031
5	1	0	2.498187	-0.332205	-1.349797
6	6	0	0.494526	-1.710016	-0.066338
7	6	0	0.405300	1.490960	-0.511805
8	1	0	1.717855	-0.923620	1.561402
9	1	0	2.524745	-2.055201	0.500676
10	1	0	2.011099	1.674170	0.913805
11	1	0	2.475837	2.036707	-0.733420
12	1	0	0.336936	-2.744876	0.265915
13	6	0	-0.744239	-0.941635	0.319828
14	6	0	-0.562750	0.966189	0.557800
15	1	0	0.164868	2.553586	-0.632354
16	1	0	0.550010	-1.739035	-1.160313
17	1	0	0.189882	1.022048	-1.479354

18	1	0	-1.195340	-1.118374	1.295298
19	1	0	-0.102302	0.835822	1.559754
20	8	0	-1.780746	1.340482	0.538939
21	8	0	-1.644858	-0.867226	-0.669146
22	8	0	-2.767008	-0.288170	-0.259484

Zero-point correction= 0.186020 (Hartree/Particle)
Thermal correction to Energy= 0.194960
Thermal correction to Enthalpy= 0.195904
Thermal correction to Gibbs Free Energy= 0.152318
Sum of electronic and zero-point Energies= -499.266757
Sum of electronic and thermal Energies= -499.257817
Sum of electronic and thermal Enthalpies= -499.256872
Sum of electronic and thermal Free Energies= -499.300459

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	122.339	35.298	91.735

Cycloheptene Primary Ozonide Syn Cycloreversion Transition Structure

SCF Done: E(RB+HF-LYP) = -499.448212874 A.U. after 1 cycles
Convg = 0.4813D-08 -V/T = 2.0091
S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.483077	-0.578641	0.146275
2	6	0	-2.490593	-0.321605	-0.243547
3	6	0	-1.994250	0.961615	0.448118
4	6	0	-1.587911	-1.556820	-0.109949
5	1	0	-2.632464	-0.097041	-1.309258
6	6	0	-0.771786	1.609432	-0.230894
7	6	0	-0.109247	-1.326945	-0.456278
8	1	0	-1.789967	0.773741	1.512027
9	1	0	-2.818193	1.684146	0.435297
10	1	0	-1.655108	-1.954220	0.912655
11	1	0	-1.978408	-2.346891	-0.761499
12	1	0	-0.826413	2.698642	-0.106996
13	6	0	0.638409	1.251807	0.280170
14	6	0	0.634375	-0.626465	0.661102
15	1	0	0.406107	-2.289585	-0.584700
16	1	0	-0.785971	1.429704	-1.310670
17	1	0	0.014797	-0.795032	-1.401563
18	1	0	0.819518	1.587224	1.321527
19	1	0	0.239599	-0.756271	1.669799
20	8	0	1.968125	-0.749606	0.709037
21	8	0	1.607695	1.366168	-0.548262
22	8	0	2.496129	-0.529298	-0.487678

```
Zero-point correction=                           0.186198 (Hartree/Particle)
Thermal correction to Energy=                    0.195065
Thermal correction to Enthalpy=                  0.196009
Thermal correction to Gibbs Free Energy=         0.152655
Sum of electronic and zero-point Energies=           -499.262015
Sum of electronic and thermal Energies=              -499.253148
Sum of electronic and thermal Enthalpies=            -499.252204
Sum of electronic and thermal Free Energies=         -499.295558

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                  122.405             35.146            91.247
```

1-Methylcyclohexene Primary Ozonide (best conformer)

```
SCF Done:  E(RB+HF-LYP) =  -499.489841128     A.U. after    7 cycles
            Convg  =    0.7236E-08             -V/T =  2.0090
            S**2   =   0.0000

                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -1.337309   -0.847938    1.049799
   2          6             0       -2.144682   -0.546682   -0.217187
   3          6             0        0.169703   -0.657879    0.858909
   4          1             0       -1.522393   -1.866802    1.406430
   5          1             0       -1.648704   -0.175096    1.860741
   6          6             0       -1.815910    0.853074   -0.751557
   7          6             0        0.589712    0.643868    0.128628
   8          1             0       -3.214997   -0.635982   -0.000779
   9          1             0       -1.908101   -1.295184   -0.982492
  10          1             0        0.684655   -0.693644    1.829318
  11          8             0        0.685483   -1.702110    0.030226
  12          6             0       -0.317745    0.977833   -1.070102
  13          1             0       -2.114964    1.608640   -0.011192
  14          1             0       -2.396199    1.064631   -1.656622
  15          8             0        1.899804    0.236998   -0.319414
  16          8             0        1.654754   -1.042287   -0.898468
  17          1             0       -0.075148    1.985297   -1.426129
  18          1             0       -0.066210    0.280540   -1.874642
  19          6             0        0.813653    1.817612    1.073800
  20          1             0        1.497634    1.544819    1.881393
  21          1             0        1.236134    2.666374    0.529462
  22          1             0       -0.136566    2.136259    1.512016
---------------------------------------------------------------------

Zero-point correction=                           0.187829 (Hartree/Particle)
Thermal correction to Energy=                    0.196889
Thermal correction to Enthalpy=                  0.197833
Thermal correction to Gibbs Free Energy=         0.154310
Sum of electronic and zero-point Energies=           -499.302012
Sum of electronic and thermal Energies=              -499.292952
```

```
Sum of electronic and thermal Enthalpies=            -499.292008
Sum of electronic and thermal Free Energies=         -499.335531

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                  123.550             36.184             91.602
```

1-Methylcyclohexane Primary Ozonide 2nd Best Syn Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -499.464310826     A.U. after   17 cycles
            Convg  =     .4734D-08             -V/T =  2.0091
            S**2   =    .0000

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -1.487715    -.759237     .980158
   2          6             0       -2.184058    -.375838    -.323652
   3          6             0         .033437    -.998468     .839937
   4          1             0       -1.899832   -1.694164    1.378036
   5          1             0       -1.655396     .005526    1.749340
   6          6             0       -1.680835     .974520    -.840400
   7          6             0         .680089     .661216     .155851
   8          1             0       -3.267588    -.337874    -.164620
   9          1             0       -1.992074   -1.154566   -1.070007
  10          1             0         .553757    -.996970    1.818735
  11          8             0         .428106   -1.848962    -.033061
  12          6             0        -.164933     .959967   -1.073022
  13          1             0       -1.954205    1.768513    -.131950
  14          1             0       -2.171607    1.226269   -1.786976
  15          8             0        1.923464     .163719    -.089174
  16          8             0        1.910391    -.790311   -1.009555
  17          1             0         .167334    1.940320   -1.443910
  18          1             0         .088501     .215313   -1.828106
  19          6             0         .756562    1.695282    1.252669
  20          1             0        1.494141    1.404225    2.003834
  21          1             0        1.040086    2.670695     .841261
  22          1             0        -.214074    1.812493    1.739431
---------------------------------------------------------------------

Zero-point correction=                           .185170 (Hartree/Particle)
Thermal correction to Energy=                    .194365
Thermal correction to Enthalpy=                  .195309
Thermal correction to Gibbs Free Energy=         .151577
Sum of electronic and zero-point Energies=          -499.279141
Sum of electronic and thermal Energies=             -499.269946
Sum of electronic and thermal Enthalpies=           -499.269001
Sum of electronic and thermal Free Energies=        -499.312733

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
```

TOTAL	121.966	36.319	92.042

1-Methylcyclohexane Primary Ozonide Worst Syn Cycloreversion Transition Structure

SCF Done: E(RB+HF-LYP) = -499.462209668 A.U. after 5 cycles
Convg = .7905D-08 -V/T = 2.0091
S**2 = .0000

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.029540	1.455321	-.070422
2	6	-2.112156	.542943	.495937
3	6	.428016	.928505	.096856
4	1	-1.041267	2.428757	.434750
5	1	-1.212898	1.653064	-1.134200
6	6	-2.174591	-.776898	-.277564
7	6	.322129	-.708433	-.806583
8	1	-3.080921	1.053171	.448503
9	1	-1.897433	.346158	1.551903
10	8	.765128	.534509	1.275841
11	6	-.827962	-1.505546	-.229668
12	1	-2.464376	-.581163	-1.319713
13	1	-2.945208	-1.433336	.140748
14	1	.295774	-.494594	-1.877034
15	8	1.577399	-1.100787	-.480780
16	8	1.683082	-1.308586	.826874
17	1	-.878187	-2.440788	-.805114
18	1	-.570330	-1.758867	.798898
19	6	1.463905	1.771397	-.661470
20	1	1.491715	2.772446	-.216744
21	1	2.455170	1.328301	-.555811
22	1	1.224276	1.882027	-1.724181

Zero-point correction= .185121 (Hartree/Particle)
Thermal correction to Energy= .194318
Thermal correction to Enthalpy= .195262
Thermal correction to Gibbs Free Energy= .151598
Sum of electronic and zero-point Energies= -499.277089
Sum of electronic and thermal Energies= -499.267892
Sum of electronic and thermal Enthalpies= -499.266948
Sum of electronic and thermal Free Energies= -499.310611

	E KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	121.936	36.471	91.898

1-Methylcyclohexane Primary Ozonide Best Syn Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -499.466569316     A.U. after    4 cycles
            Convg  =     .6146D-08             -V/T =  2.0091
            S**2   =    .0000

                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          6            .791890   -1.560008    -.134074
   2          6           1.992484    -.853731     .512407
   3          6           -.489312    -.744238    -.140744
   4          1            .587928   -2.519530     .360193
   5          1           1.026012   -1.798003   -1.178056
   6          6           2.303843     .482534    -.173109
   7          6           -.167191    1.016851    -.690802
   8          1           2.860351   -1.520331     .456585
   9          1           1.791529    -.684276    1.576569
  10          8           -.843341    -.375500    1.121254
  11          6           1.146344    1.481423    -.055619
  12          1           2.536000     .302258   -1.233179
  13          1           3.207385     .920906     .265153
  14          1           -.090359     .723169   -1.757289
  15          8          -1.249929    1.623177    -.356631
  16          8          -1.949416     .364031    1.112515
  17          1           1.417856    2.432655    -.531346
  18          1            .935627    1.706588     .995356
  19          6          -1.618849   -1.222221   -1.027717
  20          1          -2.096345   -2.088617    -.554782
  21          1          -2.365112    -.441395   -1.159808
  22          1          -1.224643   -1.530740   -1.998544
---------------------------------------------------------------------

Zero-point correction=                           .184869 (Hartree/Particle)
Thermal correction to Energy=                    .194041
Thermal correction to Enthalpy=                  .194985
Thermal correction to Gibbs Free Energy=         .151383
Sum of electronic and zero-point Energies=          -499.281701
Sum of electronic and thermal Energies=             -499.272529
Sum of electronic and thermal Enthalpies=           -499.271585
Sum of electronic and thermal Free Energies=        -499.315186

                     E                     CV                    S
                  KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL               121.762             36.404             91.768
```

1-Methylcyclohexane Primary Ozonide Anti Cycloreversion Transition Structure

```
SCF Done:  E(RB+HF-LYP) =  -499.462156815     A.U. after   18 cycles
            Convg  =     .2481D-08             -V/T =  2.0091
```

```
            S**2   =    .0000

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -1.103079   -1.176146     .977767
   2          6             0       -2.041907    -.879674    -.202325
   3          6             0         .335810    -.815025     .708894
   4          1             0       -1.152103   -2.236309    1.259953
   5          1             0       -1.420740    -.611003    1.860954
   6          6             0       -2.002597     .598906    -.608063
   7          6             0         .532759     .951182    -.022686
   8          1             0       -3.060621   -1.169470     .077582
   9          1             0       -1.758839   -1.504173   -1.057984
  10          1             0        1.013084    -.677509    1.550507
  11          8             0         .896716   -1.479047    -.309757
  12          6             0        -.607857    1.055389   -1.059686
  13          1             0       -2.354236    1.217625     .228943
  14          1             0       -2.711370     .767909   -1.426905
  15          8             0        1.721600     .890520    -.507008
  16          8             0        2.170757   -1.123333    -.452377
  17          6             0         .383966    1.802182    1.254908
  18          1             0        -.649208    2.105559   -1.378601
  19          1             0        -.285050     .477363   -1.931681
  20          1             0        1.254266    1.652656    1.897137
  21          1             0         .359357    2.857379     .961445
  22          1             0        -.529696    1.593962    1.818942
---------------------------------------------------------------------

Zero-point correction=                           .185108 (Hartree/Particle)
Thermal correction to Energy=                    .194321
Thermal correction to Enthalpy=                  .195265
Thermal correction to Gibbs Free Energy=         .151534
Sum of electronic and zero-point Energies=          -499.277049
Sum of electronic and thermal Energies=             -499.267836
Sum of electronic and thermal Enthalpies=           -499.266892
Sum of electronic and thermal Free Energies=        -499.310623

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                  121.938             36.558            92.040
```

Acetaldehyde

```
SCF Done:  E(RB+HF-LYP) =  -153.835726586     A.U. after    1 cycles
            Convg  =    0.7283D-09             -V/T =  2.0093
            S**2   =   0.0000

                  Standard orientation:
---------------------------------------------------------
Center     Atomic             Coordinates (Angstroms)
Number     Number            X           Y           Z
```

```
---------------------------------------------------------------------
   1          1          -0.503475    1.457338    0.000000
   2          6           0.000000    0.463197    0.000000
   3          8           1.208147    0.384528    0.000000
   4          6          -0.935391   -0.718648    0.000000
   5          1          -1.589203   -0.674139    0.879676
   6          1          -0.370949   -1.652574    0.000000
   7          1          -1.589203   -0.674139   -0.879676
---------------------------------------------------------------------

Zero-point correction=                           0.055589 (Hartree/Particle)
Thermal correction to Energy=                    0.059488
Thermal correction to Enthalpy=                  0.060433
Thermal correction to Gibbs Free Energy=         0.030629
Sum of electronic and zero-point Energies=           -153.780137
Sum of electronic and thermal Energies=              -153.776238
Sum of electronic and thermal Enthalpies=            -153.775294
Sum of electronic and thermal Free Energies=         -153.805098

                       E                CV                S
                    KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
TOTAL                  37.329            11.194            62.728
```

Syn acetaldehyde oxide

```
SCF Done:  E(RB+HF-LYP) =  -228.916087986     A.U. after    1 cycles
            Convg  =    0.1155D-08             -V/T =  2.0088
            S**2   =   0.0000

                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          8          -0.975131    0.042047    0.000000
   2          6           0.000000    0.858853    0.000000
   3          6           1.389456    0.375664    0.000000
   4          1          -0.310705    1.900089    0.000000
   5          8          -0.675625   -1.285314    0.000000
   6          1           2.104897    1.198126    0.000000
   7          1           1.537558   -0.279593    0.868873
   8          1           1.537558   -0.279593   -0.868873
---------------------------------------------------------------------

Zero-point correction=                           0.059574 (Hartree/Particle)
Thermal correction to Energy=                    0.064065
Thermal correction to Enthalpy=                  0.065009
Thermal correction to Gibbs Free Energy=         0.032976
Sum of electronic and zero-point Energies=           -228.856514
Sum of electronic and thermal Energies=              -228.852023
Sum of electronic and thermal Enthalpies=            -228.851079
Sum of electronic and thermal Free Energies=         -228.883112

                       E                CV                S
```

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	40.201	14.387	67.419

Anti Acetaldehyde Oxide

SCF Done: E(RB+HF-LYP) = -228.911201878 A.U. after 1 cycles
Convg = 0.9136D-09 -V/T = 2.0087
S**2 = 0.0000

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.153635	-0.690770	0.000000
2	6	0.000000	0.567265	0.000000
3	8	1.411676	-1.200371	0.000000
4	6	-1.375001	1.121559	0.000000
5	1	0.908722	1.167962	0.000000
6	1	-2.111595	0.315975	0.000000
7	1	-1.534801	1.756122	0.880832
8	1	-1.534801	1.756122	-0.880832

Zero-point correction= 0.059367 (Hartree/Particle)
Thermal correction to Energy= 0.064088
Thermal correction to Enthalpy= 0.065032
Thermal correction to Gibbs Free Energy= 0.032670
Sum of electronic and zero-point Energies= -228.851835
Sum of electronic and thermal Energies= -228.847114
Sum of electronic and thermal Enthalpies= -228.846169
Sum of electronic and thermal Free Energies= -228.878532

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	40.216	14.730	68.113