mesmer-input.txt

Mesmer Input Files


*************************************** CH3OCH2OO

```xml
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>CH3OCH2_O2_with_Internal_Rotations</me:title>
  <moleculeList>
    <molecule id="O2" description="oxygen">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">1.597738</array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>2</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">1770.2010</array>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">32</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
          <scalar>3</scalar>
        </property>
      </propertyList>
      <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
    </molecule>
     <molecule id="N0" description="nitrogen">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">1.875414685</array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>2</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">2074.7931</array>
        </property>
```

```xml
      <property dictRef="me:MW">
        <scalar units="amu">30</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
  <molecule id="CH3OCH2" description="radical">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kJ/mol">0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">
              1.590988519
              0.361313349
              0.313224621
        </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">
              180.2479
              290.5574
              444.3161
              585.9479
              1006.8570
              1148.2030
              1182.9000
              1268.2200
              1324.3820
              1465.3290
              1503.5930
              1507.1000
              1516.8220
              3036.3100
              3100.8430
              3135.9670
              3168.7300
              3281.3070
        </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">45</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:epsilon">
```

```
        <scalar>373</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>4.73</scalar>
      </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
      <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod name="ClassicalRotors"/>
  </molecule>
  <molecule id="CH3OCH2OO" description="ROO">
 <atomArray>
 <atom id="a1" elementType="C" x3="-0.914308" y3="0.540811" z3="-0.435651"/>
 <atom id="a2" elementType="O" x3="-0.290166" y3="-0.673833" z3="-0.397205"/>
 <atom id="a3" elementType="O" x3="0.037170" y3="1.623803" z3="-0.303507"/>
 <atom id="a4" elementType="O" spinMultiplicity="2" x3="0.207445" y3="1.957757"
z3="0.941003"/>
 <atom id="a5" elementType="C" x3="0.211860" y3="-1.041661" z3="0.877854"/>
 <atom id="a6" elementType="H" x3="-1.639485" y3="0.675870" z3="0.371212"/>
 <atom id="a7" elementType="H" x3="-1.348760" y3="0.668478" z3="-1.423591"/>
 <atom id="a8" elementType="H" x3="0.510674" y3="-2.083115" z3="0.803973"/>
 <atom id="a9" elementType="H" x3="-0.561814" y3="-0.929918" z3="1.641627"/>
 <atom id="a10" elementType="H" x3="1.073009" y3="-0.431121" z3="1.151755"/>
 </atomArray>
 <bondArray>
 <bond atomRefs2="a7 a1" order="1"/>
 <bond atomRefs2="a1 a2" order="1"/>
 <bond id="b1" atomRefs2="a1 a3" order="1"/>
 <bond atomRefs2="a1 a6" order="1"/>
 <bond id="b2" atomRefs2="a2 a5" order="1"/>
 <bond atomRefs2="a3 a4" order="1"/>
 <bond atomRefs2="a8 a5" order="1"/>
 <bond atomRefs2="a5 a10" order="1"/>
 <bond atomRefs2="a5 a9" order="1"/>
 </bondArray>
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kJ/mol">-145.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">
            0.325453424
            0.137159785
            0.106390236
        </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">
            214.8518
```

```
                    398.6693
                    474.5316
                    604.6601
                    919.4032
                    993.3748
                    1137.8660
                    1182.2540
                    1203.4900
                    1263.1670
                    1291.1490
                    1343.3430
                    1424.3930
                    1477.0400
                    1493.6760
                    1506.9690
                    1520.7800
                    3043.6200
                    3082.8600
                    3117.8830
                    3162.0370
                    3183.4200
            </array>
        </property>
        <property dictRef="me:MW">
            <scalar units="amu">77</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
            <scalar>2</scalar>
        </property>
        <property dictRef="me:eletronicExcitation">
            <array units="cm-1">0</array>
        </property>
        <property dictRef="me:epsilon">
            <scalar>373</scalar>
        </property>
        <property dictRef="me:sigma">
            <scalar>6.07</scalar>
        </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
        <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod name="ClassicalRotors"/>
    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
        <me:bondRef>b1</me:bondRef>
        <me:HinderedRotorPotential format="numerical" units="kJ/mol"
expansionSize="7" scale="1" UseSineTerms="yes">
            <me:PotentialPoint angle= "0.0" potential= "14.1334" />
            <me:PotentialPoint angle= "10.0" potential= "13.2162" />
            <me:PotentialPoint angle= "20.0" potential= "11.6421" />
            <me:PotentialPoint angle= "30.0" potential= "9.6274" />
            <me:PotentialPoint angle= "40.0" potential= "7.6480" />
            <me:PotentialPoint angle= "50.0" potential= "5.7252" />
            <me:PotentialPoint angle= "60.0" potential= "4.1568" />
            <me:PotentialPoint angle= "70.0" potential= "3.2440" />
            <me:PotentialPoint angle= "80.0" potential= "3.3164" />
```

```xml
          <me:PotentialPoint angle= "90.0" potential= "4.2725" />
          <me:PotentialPoint angle= "100.0" potential= "5.5832" />
          <me:PotentialPoint angle= "110.0" potential= "7.1123" />
          <me:PotentialPoint angle= "120.0" potential= "7.9283" />
          <me:PotentialPoint angle= "130.0" potential= "8.2733" />
          <me:PotentialPoint angle= "140.0" potential= "8.0165" />
          <me:PotentialPoint angle= "150.0" potential= "7.1359" />
          <me:PotentialPoint angle= "160.0" potential= "5.9852" />
          <me:PotentialPoint angle= "170.0" potential= "4.8809" />
          <me:PotentialPoint angle= "180.0" potential= "4.1512" />
          <me:PotentialPoint angle= "190.0" potential= "3.8985" />
          <me:PotentialPoint angle= "200.0" potential= "4.0402" />
          <me:PotentialPoint angle= "210.0" potential= "4.2240" />
          <me:PotentialPoint angle= "220.0" potential= "4.1973" />
          <me:PotentialPoint angle= "230.0" potential= "3.7980" />
          <me:PotentialPoint angle= "240.0" potential= "2.8950" />
          <me:PotentialPoint angle= "250.0" potential= "1.6915" />
          <me:PotentialPoint angle= "260.0" potential= "0.4901" />
          <me:PotentialPoint angle= "270.0" potential= "0.0" />
          <me:PotentialPoint angle= "280.0" potential= "0.7919" />
          <me:PotentialPoint angle= "290.0" potential= "2.7001" />
          <me:PotentialPoint angle= "300.0" potential= "5.1737" />
          <me:PotentialPoint angle= "310.0" potential= "7.6800" />
          <me:PotentialPoint angle= "320.0" potential= "10.1040" />
          <me:PotentialPoint angle= "330.0" potential= "13.8251" />
          <me:PotentialPoint angle= "340.0" potential= "13.6838" />
          <me:PotentialPoint angle= "350.0" potential= "14.2930" />
          <me:PotentialPoint angle= "360.0" potential= "14.1334" />
        </me:HinderedRotorPotential>
        <me:periodicity>1</me:periodicity>
    </me:ExtraDOSCMethod>
    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
        <me:bondRef>b2</me:bondRef>
        <me:HinderedRotorPotential format="analytical" units="kJ/mol">
          <me:PotentialPoint index="0"  coefficient="3.89" />
          <me:PotentialPoint index="3"  coefficient="-3.89" />
        </me:HinderedRotorPotential>
        <me:periodicity>3</me:periodicity>
    </me:ExtraDOSCMethod>
</molecule>
    <molecule id="CH2OCH2OOH">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kJ/mol">-105.5</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">
             0.343345605
             0.125450032
             0.114002935
      </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
```

```
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">
            83.6909
           200.4650
           277.9852
           315.1313
           371.9879
           480.7373
           533.4745
           669.1102
           966.8152
          1006.5010
          1123.5130
          1137.5360
          1234.6950
          1276.1530
          1332.2140
          1431.2720
          1443.5390
          1481.8310
          1508.7240
          3087.7050
          3159.5390
          3169.4050
          3301.8900
          3797.4600
      </array>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">77</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>373</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>6.07</scalar>
    </property>
  </propertyList>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
  </me:energyTransferModel>
  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
<molecule id="TS_H_shift">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kJ/mol">-59.3</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">
           0.290444891
```

```
                0.177124954
                0.12193341
      </array>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">
          259.9200
          415.9508
          480.6133
          495.0158
          599.3272
          710.1579
          966.2378
          1011.7750
          1089.3470
          1143.2910
          1162.6650
          1219.3700
          1222.5620
          1275.7930
          1320.9710
          1411.3090
          1484.8020
          1504.5240
          1670.8700
          3067.0520
          3075.9860
          3187.9590
          3220.3200
      </array>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">77</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">
      <scalar units="cm-1">1868.4</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
<molecule id="OOCH2OCH2OOH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kJ/mol">-250</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">
```

```
0.157444374
0.070631983
0.054923849
        </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">
81.9261
105.0616
155.0602
226.9255
314.251
372.3583
424.2656
456.0055
528.59
682.9059
963.6882
981.4374
1018.727
1106.512
1134.017
1184.574
1234.109
1289.467
1314.044
1330.885
1411.263
1439.189
1462.25
1490.188
1517.613
3090.145
3096.316
3170.854
3180.728
3779.973
        </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">109</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
   <molecule id="CH3OCH2O">
     <propertyList>
```

```
      <property dictRef="me:ZPE">
        <scalar units="kJ/mol">-300</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">
0.671364352
0.212764494
0.180484351
        </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">
145.6126
209.068
365.3598
613.4597
809.2092
976.2433
1077.506
1150.24
1185.712
1225.023
1270.586
1352.573
1398.154
1484.292
1500.532
1520.514
2899.05
3026.579
3030.3
3104.304
3157.224
        </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">61</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
  <molecule id="N2">
    <atom elementType="He" />
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
      </property>
```

```
      <property dictRef="me:sigma">
        <scalar>3.9</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">28.0</scalar>
      </property>
    </propertyList>
  </molecule>
</moleculeList>
<reactionList>
  <reaction id="R_00">
    <reactant>
      <molecule ref="CH3OCH2" role="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="O2" role="excessReactant" />
    </reactant>
    <product>
      <molecule ref="CH3OCH2OO" role="modelled" />
    </product>
    <me:MCRCMethod xsi:type="me:MesmerILT">
      <me:preExponential units="cm3molecule-1s-1">6.00e-12</me:preExponential>
      <me:activationEnergy units="kJ/mol">0.0</me:activationEnergy>
      <me:TInfinity>298.0</me:TInfinity>
      <me:nInfinity>0.00000000001</me:nInfinity>
    </me:MCRCMethod>
    <me:excessReactantConc>5E18</me:excessReactantConc>
  </reaction>
    <reaction id="H_shift">
    <reactant>
      <molecule ref="CH3OCH2OO" role="modelled" />
    </reactant>
    <product>
      <molecule ref="CH2OCH2OOH" role="modelled" />
    </product>
    <me:transitionState>
      <molecule ref="TS_H_shift" role="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
  <reaction id="CH2OCH2OOH_OOCH2CH2OOH">
    <reactant>
      <molecule ref="CH2OCH2OOH" role="modelled" />
    </reactant>
    <reactant>
      <molecule ref="O2" role="excessReactant" />
    </reactant>
    <product>
      <molecule ref="OOCH2OCH2OOH" role="sink" />
    </product>
    <me:MCRCMethod name="SimpleBimolecularSink"/>

<me:BimolecularLossRateCoefficient>6.00e-12</me:BimolecularLossRateCoefficient>
    <me:excessReactantConc>5E18</me:excessReactantConc>
  </reaction>
```

```
    <reaction id="CH3OCH2OO_CH3OOCH2O">
      <reactant>
        <molecule ref="CH3OCH2OO" role="modelled" />
      </reactant>
      <product>
        <molecule ref="CH3OCH2O" role="sink" />
      </product>
      <me:MCRCMethod xsi:type ="me:MesmerILT">
        <me:preExponential units="s-1">0.0001</me:preExponential>
        <me:activationEnergy units="kJ/mol">0.0</me:activationEnergy>
        <me:TInfinity>298.0</me:TInfinity>
        <me:nInfinity>0.00000001</me:nInfinity>
      </me:MCRCMethod>
    </reaction>
  </reactionList>
  <me:conditions>
    <me:bathGas>N2</me:bathGas>
    <me:PTs>
      <me:PTpair units="Torr" P="760.0" T="233.0" />
      <me:PTpair units="Torr" P="760.0" T="243.0" />
      <me:PTpair units="Torr" P="760.0" T="253.0" />
      <me:PTpair units="Torr" P="760.0" T="263.0" />
      <me:PTpair units="Torr" P="760.0" T="273.0" />
      <me:PTpair units="Torr" P="760.0" T="283.0" />
      <me:PTpair units="Torr" P="760.0" T="293.0" />
      <me:PTpair units="Torr" P="760.0" T="298.0" />
      <me:PTpair units="Torr" P="760.0" T="303.0" />
      <me:PTpair units="Torr" P="760.0" T="313.0" />
      <me:PTpair units="Torr" P="760.0" T="323.0" />
      <me:PTpair units="Torr" P="760.0" T="333.0" />
    </me:PTs>
    <me:InitialPopulation>
      <me:molecule ref="CH3OCH2" population="1.0" />
    </me:InitialPopulation>
  </me:conditions>
  <me:modelParameters>
    <!--Specify grain size directly...-->
    <me:grainSize units="cm-1">50</me:grainSize>
    <!--...or by the total number of grains
        <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
        <me:maxTemperature>6000</me:maxTemperature>-->
    <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
    <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
  </me:modelParameters>
  <me:control>
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
```

******************************************* HOOCH2OCH2OO

```
<?xml version="1.0" encoding="utf-8" ?>
```

```xml
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>H-Shift in OOCH2OCH2OH</me:title>
  <moleculeList>
    <molecule id="Q200">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
              0.190750
              0.104448
              0.073688
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">
              86.8670
              113.6269
              190.9687
              374.0242
              429.5281
              491.7337
              556.1609
              620.1571
              890.0228
              968.3785
              1061.4826
              1154.5877
              1159.3329
              1206.0769
              1295.0611
              1318.7591
              1348.5231
              1403.7202
              1433.4829
              1462.1099
              1494.8781
              1524.8097
              3050.9384
              3086.2677
              3163.4672
              3181.3714
              3859.9650
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        </property>
```

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    </property>
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    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
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          230.2992
          376.0804
          428.9020
          450.6814
          509.9408
          534.6098
          695.4711
          990.6678
          1001.0533
          1061.7271
          1108.6146
          1148.5009
          1201.5196
          1219.1640
          1300.4416
          1319.7670
          1352.6175
```

```
                    1402.3178
                    1432.2788
                    1504.0727
                    1678.7658
                    3079.5749
                    3084.1211
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0.070631983
0.054923849
        </array>
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      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
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        <array units="cm-1">
81.9261
105.0616
155.0602
226.9255
314.251
372.3583
424.2656
456.0055
528.59
682.9059
963.6882
981.4374
1018.727
1106.512
```

```
1134.017
1184.574
1234.109
1289.467
1314.044
1330.885
1411.263
1439.189
1462.25
1490.188
1517.613
3090.145
3096.316
3170.854
3180.728
3779.973
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        <property dictRef="me:sigma">
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        </property>
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        </property>
      </propertyList>
    </molecule>
  </moleculeList>
  <reactionList>
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        <molecule ref="Q200" role="modelled" />
      </reactant>
      <product>
        <molecule ref="Product" role="sink" />
      </product>
      <me:transitionState>
        <molecule ref="TS_H_shift" role="transitionState" />
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
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        </me:PTs>
        <me:InitialPopulation>
          <me:molecule ref="Q200" population="1.0" />
        </me:InitialPopulation>
      </me:conditions>
      <me:modelParameters>
        <!--Specify grain size directly...-->
        <me:grainSize units="cm-1">50</me:grainSize>
        <!--...or by the total number of grains
            <me:numberOfGrains> 500 </me:numberOfGrains>-->
        <!--Specify increased energy range
            <me:maxTemperature>6000</me:maxTemperature>-->
        <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
        <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
      </me:modelParameters>
      <me:control>
        <me:printSpeciesProfile />
        <me:testRateConstants />
        <me:eigenvalues>10</me:eigenvalues>
      </me:control>
</me:mesmer>



************************************* CH3CH2OCH(OO)CH3

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen' ?>
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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
           xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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         </property>
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                </property>
                <property dictRef="me:frequenciesScaleFactor">
                    <scalar>0.974</scalar>
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                </property>
                <property dictRef="me:MW">
                    <scalar units="amu">32</scalar>
                </property>
                <property dictRef="me:spinMultiplicity">
                    <scalar>3</scalar>
                </property>
            </propertyList>
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        </molecule>
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     <atom id="a2" elementType="H" x3="-3.742364" y3="0.757078" z3="0.136000"/>
     <atom id="a3" elementType="H" x3="-3.239661" y3="-0.922953" z3="0.377072"/>
     <atom id="a4" elementType="H" x3="-3.061103" y3="-0.165124" z3="-1.209729"/>
     <atom id="a5" elementType="C" x3="1.426332" y3="-1.540335" z3="-0.079832"/>
     <atom id="a6" elementType="H" x3="1.384326" y3="-1.705879" z3="-1.154851"/>
     <atom id="a7" elementType="H" x3="2.460233" y3="-1.392030" z3="0.223036"/>
     <atom id="a8" elementType="H" x3="1.020195" y3="-2.412006" z3="0.427726"/>
     <atom id="a9" elementType="O" x3="-0.689584" y3="-0.521029" z3="-0.155260"/>
     <atom id="a10" elementType="C" x3="-1.618296" y3="0.484064" z3="0.239414"/>
     <atom id="a11" elementType="H" x3="-1.377295" y3="1.423935" z3="-0.262340"/>
     <atom id="a12" elementType="H" x3="-1.530183" y3="0.649524" z3="1.318176"/>
     <atom id="a13" elementType="C" x3="0.601033" y3="-0.333135" z3="0.270254"/>
     <atom id="a14" elementType="H" x3="0.646392" y3="-0.048026" z3="1.325648"/>
     <atom id="a15" elementType="O" x3="1.193274" y3="0.794453" z3="-0.444847"/>
     <atom id="a16" elementType="O" spinMultiplicity="2" x3="1.023183"
y3="1.914821" z3="0.187240"/>
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    <bondArray>
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     <bond atomRefs2="a6 a5" order="1"/>
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     <bond id="b1" atomRefs2="a15 a13" order="1"/>
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              0.061499
              0.044368
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              121.2364
              187.5063
              193.7338
              244.2257
              309.8345
              383.5848
              434.3606
              564.6068
              573.5548
              825.5156
              838.4426
              883.1230
              978.9133
              1082.0757
              1111.4718
              1149.1391
              1183.4632
              1196.4912
              1232.5739
              1302.3129
              1314.6608
              1367.8583
              1384.5968
              1410.1447
              1424.9672
              1459.7787
              1484.7027
              1487.3435
              1493.8855
              1506.9663
              1531.6426
              3039.0902
              3060.0719
              3069.8457
              3087.2472
```

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                3090.4208
                3136.3489
                3143.0042
                3155.2943
                3157.8574
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      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
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      <property dictRef="me:epsilon">
        <scalar>504.0</scalar>
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      <property dictRef="me:sigma">
        <scalar>6.2</scalar>
      </property>
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      <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
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      <me:bondRef>b1</me:bondRef>
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expansionSize="7" scale="1" UseSineTerms="yes">
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        <me:PotentialPoint angle= "140.0" potential= "2.1384" />
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            0.044540
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      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
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            193.9082
            202.7631
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            295.5356
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            387.0963
            437.5673
            562.4603
            612.1208
            647.5250
            878.2801
            907.4239
            992.2094
            1030.4092
            1058.6802
            1131.3668
            1138.2802
```

```
                    1179.1487
                    1203.8063
                    1263.5924
                    1374.1457
                    1375.0821
                    1404.1305
                    1425.3855
                    1445.4602
                    1457.1092
                    1471.8306
                    1488.0610
                    1493.7136
                    1498.1220
                    3004.1078
                    3072.9646
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                    3088.2110
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                    3156.4185
                    3162.9007
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      </property>
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        <scalar>6.2</scalar>
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            0.068153
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        <scalar>1</scalar>
```

```
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        211.7029
        216.9508
        287.2305
        321.7896
        419.1738
        473.0825
        502.3432
        572.9773
        633.3922
        860.1020
        882.7649
        901.1426
        977.1351
        1083.4926
        1112.3210
        1141.8928
        1156.2423
        1174.7304
        1197.7811
        1230.4898
        1288.3172
        1358.3962
        1381.3022
        1400.0735
        1423.1998
        1450.3595
        1485.8031
        1490.9374
        1493.1370
        1496.3652
        1660.9617
        3052.5649
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        3082.2962
        3123.4977
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        3160.6567
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    <property dictRef="me:ZPE">
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0.070631983
0.054923849
      </array>
    </property>
    <property dictRef="me:symmetryNumber">
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      <scalar>0.974</scalar>
    </property>
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81.9261
105.0616
155.0602
226.9255
314.251
372.3583
424.2656
456.0055
528.59
682.9059
963.6882
981.4374
1018.727
1106.512
1134.017
1184.574
1234.109
1289.467
1314.044
1330.885
1411.263
1439.189
1462.25
1490.188
1517.613
3090.145
3096.316
3170.854
3180.728
3779.973
      </array>
```

```xml
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        <molecule ref="Q200H" role="modelled" />
      </product>
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        <molecule ref="TS_H_shift" role="transitionState" />
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      <me:MCRCMethod name="SimpleRRKM"/>
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      <reactant>
        <molecule ref="O2" role="excessReactant" />
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```
      <me:bathGas>N2</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760.0" T="253.0" />
        <me:PTpair units="Torr" P="760.0" T="243.0" />
        <me:PTpair units="Torr" P="760.0" T="233.0" />
      </me:PTs>
      <me:InitialPopulation>
        <me:molecule ref="R200" population="1.0" />
      </me:InitialPopulation>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">50</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
      <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
    </me:modelParameters>
    <me:control>
      <me:printSpeciesProfile />
      <me:testRateConstants />
      <me:eigenvalues>10</me:eigenvalues>
    </me:control>
</me:mesmer>


********************************************* CH3CH(OO)OCH(OOH)CH3 #1

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other' ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen' ?>
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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>H-Shift in CH3CH(OOH)OCH(OO)CH3</me:title>
  <moleculeList>
    <molecule id="Q200">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
              0.072562
              0.041388
              0.030294
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
```

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<property dictRef="me:vibFreqs">
  <array units="cm-1">
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        138.5893
        163.1465
        200.1488
        213.0966
        216.2125
        281.1213
        297.7229
        328.0291
        372.8364
        421.9599
        506.9125
        553.6286
        582.9660
        644.4987
        842.3787
        878.4184
        921.6195
        996.7873
        1055.4422
        1090.7816
        1143.9527
        1145.6195
        1181.8326
        1217.6162
        1226.3336
        1308.6640
        1362.5830
        1363.6281
        1384.9361
        1418.1962
        1422.8691
        1431.7546
        1464.4158
        1490.2161
        1490.8329
        1495.8729
        1498.5222
        3079.2633
        3079.7644
        3106.1934
        3114.9029
        3163.7431
        3164.0615
        3166.6305
        3169.5862
        3829.0399
</array>
</property>
<property dictRef="me:MW">
  <scalar units="amu">137.04500</scalar>
</property>
<property dictRef="me:spinMultiplicity">
```

```xml
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>600.0</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>6.5</scalar>
    </property>
  </propertyList>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
  </me:energyTransferModel>
  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
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  <propertyList>
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    </property>
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          0.034560
    </array>
    </property>
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    </property>
    <property dictRef="me:frequenciesScaleFactor">
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    </property>
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          122.1289
          163.5712
          211.8687
          213.5723
          242.2601
          302.7320
          315.3763
          337.2521
          379.2539
          439.2531
          444.7995
          547.0995
          567.8891
          621.4907
          669.4377
          873.7360
          903.6221
          924.0003
          1009.3175
          1061.2773
          1074.1225
```

```
                    1104.9079
                    1131.5732
                    1162.3505
                    1188.7396
                    1237.3200
                    1302.2385
                    1319.9990
                    1385.2973
                    1393.5731
                    1411.1674
                    1444.3133
                    1447.5203
                    1483.9622
                    1488.7422
                    1489.4446
                    1498.6554
                    1656.2248
                    3056.9781
                    3081.1373
                    3125.1529
                    3142.3065
                    3165.1967
                    3170.5930
                    3180.3615
                    3784.7279
        </array>
        </property>
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          <scalar units="amu">137.04500</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
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        </property>
        <property dictRef="me:imFreqs">
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        </property>
      </propertyList>
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<molecule id="TS_H_shift2">
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        <scalar units="kJ/mol">79.5</scalar>
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          <array units="cm-1">
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            0.040848
            0.038706
      </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
```

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        91.9808
       170.6601
       189.6532
       221.4629
       247.6567
       249.1933
       277.9175
       313.5042
       379.5250
       404.6801
       480.4192
       556.9841
       561.7434
       606.9626
       684.5332
       868.7816
       902.5095
       930.7396
       982.8989
      1054.9003
      1072.1275
      1102.7393
      1132.3998
      1159.8253
      1188.0102
      1199.1080
      1240.2886
      1270.5432
      1384.4133
      1391.6581
      1410.5368
      1432.5497
      1441.2263
      1486.6613
      1488.1238
      1494.3665
      1498.1785
      1683.2745
      3062.4874
      3080.6745
      3125.9381
      3141.2057
      3162.9165
      3170.0422
      3173.2205
      3808.9905
  </array>
</property>
<property dictRef="me:MW">
  <scalar units="amu">137.04500</scalar>
</property>
<property dictRef="me:spinMultiplicity">
```

```
      <scalar>2</scalar>
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    <property dictRef="me:imFreqs">
      <scalar units="cm-1">1877.94</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
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  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kJ/mol">43.9</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">
            0.072562
            0.041388
            0.030294
      </array>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">
            61.3285
            66.1563
            138.5893
            163.1465
            200.1488
            213.0966
            216.2125
            281.1213
            297.7229
            328.0291
            372.8364
            421.9599
            506.9125
            553.6286
            582.9660
            644.4987
            842.3787
            878.4184
            921.6195
            996.7873
            1055.4422
            1090.7816
            1143.9527
            1145.6195
            1181.8326
            1217.6162
            1226.3336
            1308.6640
```

```
                    1362.5830
                    1363.6281
                    1384.9361
                    1418.1962
                    1422.8691
                    1431.7546
                    1464.4158
                    1490.2161
                    1490.8329
                    1495.8729
                    1498.5222
                    3079.2633
                    3079.7644
                    3106.1934
                    3114.9029
                    3163.7431
                    3164.0615
                    3166.6305
                    3169.5862
                    3829.0399
            </array>
          </property>
          <property dictRef="me:MW">
            <scalar units="amu">137.04500</scalar>
          </property>
          <property dictRef="me:spinMultiplicity">
            <scalar>2</scalar>
          </property>
        </propertyList>
        <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
      </molecule>
      <molecule id="N2">
        <atom elementType="N2" />
        <propertyList>
          <property dictRef="me:epsilon">
            <scalar>48.0</scalar>
          </property>
          <property dictRef="me:sigma">
            <scalar>3.9</scalar>
          </property>
          <property dictRef="me:MW">
            <scalar units="amu">28.0</scalar>
          </property>
        </propertyList>
      </molecule>
    </moleculeList>
    <reactionList>
      <reaction id="H_shift2">
        <reactant>
          <molecule ref="Q200" role="modelled" />
        </reactant>
        <product>
          <molecule ref="Product" role="sink" />
        </product>
        <me:transitionState>
          <molecule ref="TS_H_shift2" role="transitionState" />
```

```
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
    <reaction id="H_shift1">
      <reactant>
        <molecule ref="Q200" role="modelled" />
      </reactant>
      <product>
        <molecule ref="Product" role="sink" />
      </product>
      <me:transitionState>
        <molecule ref="TS_H_shift1" role="transitionState" />
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
  </reactionList>
  <me:conditions>
    <me:bathGas>N2</me:bathGas>
    <me:PTs>
      <me:PTpair units="Torr" P="760.0" T="233.0" />
      <me:PTpair units="Torr" P="760.0" T="243.0" />
      <me:PTpair units="Torr" P="760.0" T="253.0" />
      <me:PTpair units="Torr" P="760.0" T="263.0" />
      <me:PTpair units="Torr" P="760.0" T="273.0" />
      <me:PTpair units="Torr" P="760.0" T="283.0" />
      <me:PTpair units="Torr" P="760.0" T="293.0" />
      <me:PTpair units="Torr" P="760.0" T="298.0" />
      <me:PTpair units="Torr" P="760.0" T="303.0" />
      <me:PTpair units="Torr" P="760.0" T="313.0" />
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    </me:PTs>
    <me:InitialPopulation>
      <me:molecule ref="Q200" population="1.0" />
    </me:InitialPopulation>
  </me:conditions>
  <me:modelParameters>
    <!--Specify grain size directly...-->
    <me:grainSize units="cm-1">50</me:grainSize>
    <!--...or by the total number of grains
        <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
        <me:maxTemperature>6000</me:maxTemperature>-->
    <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
    <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
  </me:modelParameters>
  <me:control>
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
```

*********************************** CH3CH(O)OCH(OOH)CH3 #1

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
           xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>CH3CH(OOH)OCH(O)(CH3) C1 H-Shift and CH3-Elimination</me:title>
  <moleculeList>
    <molecule id="OQ2OOH">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
              0.113080
              0.051536
              0.040002
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">
              81.3213
              147.7321
              186.0401
              190.0578
              224.2439
              233.0967
              291.8222
              337.5275
              412.4554
              419.9181
              504.4320
              541.0542
              628.9819
              726.7534
              855.5154
              896.8939
              928.9691
              972.8170
              1012.8381
              1056.5388
              1085.9773
              1136.7872
              1161.8127
              1168.6588
              1212.8959
```

```
                    1225.2796
                    1334.4671
                    1385.4392
                    1389.4599
                    1405.1890
                    1432.8877
                    1476.8513
                    1485.9388
                    1487.7974
                    1495.3575
                    1498.3543
                    2974.7223
                    3053.1704
                    3080.2774
                    3080.4371
                    3159.5888
                    3169.1143
                    3172.6291
                    3177.6779
                    3757.5588
          </array>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">121.05008</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
          <scalar>2</scalar>
        </property>
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          <scalar>600.0</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>6.2</scalar>
        </property>
      </propertyList>
      <me:energyTransferModel xsi:type="me:ExponentialDown">
        <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
      </me:energyTransferModel>
      <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
    </molecule>
    <molecule id="P1D">
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          <scalar units="kJ/mol">-40.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
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              0.051536
              0.040002
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
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```
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<property dictRef="me:vibFreqs">
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         186.0401
         190.0578
         224.2439
         233.0967
         291.8222
         337.5275
         412.4554
         419.9181
         504.4320
         541.0542
         628.9819
         726.7534
         855.5154
         896.8939
         928.9691
         972.8170
        1012.8381
        1056.5388
        1085.9773
        1136.7872
        1161.8127
        1168.6588
        1212.8959
        1225.2796
        1334.4671
        1385.4392
        1389.4599
        1405.1890
        1432.8877
        1476.8513
        1485.9388
        1487.7974
        1495.3575
        1498.3543
        2974.7223
        3053.1704
        3080.2774
        3080.4371
        3159.5888
        3169.1143
        3172.6291
        3177.6779
        3757.5588
</array>
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<property dictRef="me:MW">
   <scalar units="amu">121.05008</scalar>
</property>
<property dictRef="me:spinMultiplicity">
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```

```
      </property>
      <property dictRef="me:epsilon">
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      </property>
      <property dictRef="me:sigma">
        <scalar>6.2</scalar>
      </property>
    </propertyList>
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      <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
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      </property>
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            0.051536
            0.040002
        </array>
      </property>
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        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
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      </property>
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        <array units="cm-1">
            81.3213
            147.7321
            186.0401
            190.0578
            224.2439
            233.0967
            291.8222
            337.5275
            412.4554
            419.9181
            504.4320
            541.0542
            628.9819
            726.7534
            855.5154
            896.8939
            928.9691
            972.8170
            1012.8381
            1056.5388
            1085.9773
            1136.7872
            1161.8127
```

```
                1168.6588
                1212.8959
                1225.2796
                1334.4671
                1385.4392
                1389.4599
                1405.1890
                1432.8877
                1476.8513
                1485.9388
                1487.7974
                1495.3575
                1498.3543
                2974.7223
                3053.1704
                3080.2774
                3080.4371
                3159.5888
                3169.1143
                3172.6291
                3177.6779
                3757.5588
      </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">121.05008</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
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        <scalar>600.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>6.2</scalar>
      </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
      <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
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        <scalar units="kJ/mol">31.3</scalar>
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        <scalar>1</scalar>
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        205.5729
        215.1742
        229.9967
        305.4945
        347.8756
        371.0267
        430.4654
        552.3735
        574.1671
        606.8662
        677.7788
        865.1350
        887.8024
        920.5906
        974.0203
        1083.9661
        1099.2949
        1115.1611
        1131.2427
        1171.6691
        1183.9540
        1209.9377
        1271.0029
        1317.2085
        1355.2605
        1379.8458
        1396.7917
        1412.0251
        1443.4429
        1478.4761
        1491.3376
        1493.9695
        1497.3249
        1579.6098
        3008.9314
        3060.1197
        3070.8561
        3077.4370
        3157.1792
        3160.6368
        3166.8324
        3167.2028
</array>
</property>
<property dictRef="me:MW">
  <scalar units="amu">121.05008</scalar>
</property>
<property dictRef="me:spinMultiplicity">
```

```
      <scalar>2</scalar>
    </property>
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      <scalar units="cm-1">1975.92</scalar>
    </property>
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</molecule>
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      <scalar units="kJ/mol">36.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
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          0.056876
          0.045403
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    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">
          80.7994
          118.1175
          179.4819
          190.3294
          226.4558
          242.3969
          272.8892
          345.0315
          365.7728
          422.5094
          524.6355
          561.1341
          599.9301
          684.6310
          716.6132
          811.6147
          872.8773
          901.9920
          971.9681
          1067.9722
          1100.2114
          1110.9142
          1148.4610
          1184.1465
          1199.3608
          1358.5062
          1375.8473
          1396.1828
```

```
                        1428.5742
                        1430.1119
                        1445.3732
                        1489.6167
                        1495.4406
                        1513.6317
                        1575.1015
                        3053.7983
                        3076.2663
                        3102.2217
                        3131.3146
                        3157.1305
                        3171.4552
                        3261.4565
                        3276.8868
                        3628.0965
        </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">121.05008</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:imFreqs">
        <scalar units="cm-1">515.831</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
  <molecule id="N2">
    <atom elementType="N2" />
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      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
      </property>
      <property dictRef="me:sigma">
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      </property>
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        <scalar units="amu">28.0</scalar>
      </property>
    </propertyList>
  </molecule>
</moleculeList>
<reactionList>
  <reaction id="Decomp">
    <reactant>
      <molecule ref="OQ2OOH" role="modelled" />
    </reactant>
    <product>
      <molecule ref="P1D" role="sink" />
    </product>
    <me:transitionState>
      <molecule ref="TS_D" role="transitionState" />
    </me:transitionState>
```

```
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
    <reaction id="H_Shift">
      <reactant>
        <molecule ref="OQ2OOH" role="modelled" />
      </reactant>
      <product>
        <molecule ref="P1H" role="sink" />
      </product>
      <me:transitionState>
        <molecule ref="TS_H" role="transitionState" />
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
  </reactionList>
  <me:conditions>
    <me:bathGas>N2</me:bathGas>
    <me:PTs>
      <me:PTpair units="Torr" P="760.0" T="233.0" />
      <me:PTpair units="Torr" P="760.0" T="243.0" />
      <me:PTpair units="Torr" P="760.0" T="253.0" />
      <me:PTpair units="Torr" P="760.0" T="263.0" />
      <me:PTpair units="Torr" P="760.0" T="273.0" />
      <me:PTpair units="Torr" P="760.0" T="283.0" />
      <me:PTpair units="Torr" P="760.0" T="293.0" />
      <me:PTpair units="Torr" P="760.0" T="298.15" />
      <me:PTpair units="Torr" P="760.0" T="303.0" />
      <me:PTpair units="Torr" P="760.0" T="313.0" />
      <me:PTpair units="Torr" P="760.0" T="323.0" />
      <me:PTpair units="Torr" P="760.0" T="333.0" />
      <me:PTpair units="Torr" P="760.0" T="343.0" />
    </me:PTs>
    <me:InitialPopulation>
      <me:molecule ref="OQ2OOH" population="1.0" />
    </me:InitialPopulation>
  </me:conditions>
  <me:modelParameters>
    <!--Specify grain size directly...-->
    <me:grainSize units="cm-1">50</me:grainSize>
    <!--...or by the total number of grains
        <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
        <me:maxTemperature>6000</me:maxTemperature>-->
    <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
    <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
  </me:modelParameters>
  <me:control>
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
```

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>CH3CH(OOH)OCH(O)(CH3) C2 H-Shift and CH3-Elimination</me:title>
  <moleculeList>
    <molecule id="OQ2OOH">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
              0.096161
              0.056844
              0.041315
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">
              71.5058
              122.6232
              178.2634
              196.6931
              216.5016
              227.7713
              293.7058
              355.6289
              369.6546
              438.0236
              487.0654
              548.3689
              589.5557
              707.0103
              844.1016
              897.0117
              921.2124
              950.8226
              1045.7560
              1057.0927
              1076.3442
              1132.9594
              1141.6248
              1170.1363
              1208.1227
              1224.7958
```

```
                    1351.4963
                    1371.0123
                    1393.5908
                    1410.6766
                    1424.4650
                    1478.5961
                    1483.2646
                    1485.1582
                    1495.0714
                    1504.2906
                    2984.9587
                    3065.2043
                    3077.4483
                    3122.4968
                    3145.6872
                    3154.1806
                    3167.8936
                    3171.8257
                    3737.0407
      </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">121.05008</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:epsilon">
        <scalar>600.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>6.2</scalar>
      </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
      <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
<molecule id="P1D">
    <propertyList>
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        <scalar units="kJ/mol">-40.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">
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            0.051536
            0.040002
        </array>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
```

```
</property>
<property dictRef="me:vibFreqs">
  <array units="cm-1">
        81.3213
       147.7321
       186.0401
       190.0578
       224.2439
       233.0967
       291.8222
       337.5275
       412.4554
       419.9181
       504.4320
       541.0542
       628.9819
       726.7534
       855.5154
       896.8939
       928.9691
       972.8170
      1012.8381
      1056.5388
      1085.9773
      1136.7872
      1161.8127
      1168.6588
      1212.8959
      1225.2796
      1334.4671
      1385.4392
      1389.4599
      1405.1890
      1432.8877
      1476.8513
      1485.9388
      1487.7974
      1495.3575
      1498.3543
      2974.7223
      3053.1704
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      3080.4371
      3159.5888
      3169.1143
      3172.6291
      3177.6779
      3757.5588
</array>
</property>
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  <scalar units="amu">121.05008</scalar>
</property>
<property dictRef="me:spinMultiplicity">
  <scalar>2</scalar>
</property>
```

```xml
    <property dictRef="me:epsilon">
      <scalar>600.0</scalar>
    </property>
    <property dictRef="me:sigma">
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  </me:energyTransferModel>
  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
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      <scalar units="kJ/mol">-40.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">
          0.113080
          0.051536
          0.040002
      </array>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.974</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">
          81.3213
          147.7321
          186.0401
          190.0578
          224.2439
          233.0967
          291.8222
          337.5275
          412.4554
          419.9181
          504.4320
          541.0542
          628.9819
          726.7534
          855.5154
          896.8939
          928.9691
          972.8170
          1012.8381
          1056.5388
          1085.9773
          1136.7872
          1161.8127
          1168.6588
```

```
                        1212.8959
                        1225.2796
                        1334.4671
                        1385.4392
                        1389.4599
                        1405.1890
                        1432.8877
                        1476.8513
                        1485.9388
                        1487.7974
                        1495.3575
                        1498.3543
                        2974.7223
                        3053.1704
                        3080.2774
                        3080.4371
                        3159.5888
                        3169.1143
                        3172.6291
                        3177.6779
                        3757.5588
       </array>
       </property>
       <property dictRef="me:MW">
         <scalar units="amu">121.05008</scalar>
       </property>
       <property dictRef="me:spinMultiplicity">
         <scalar>2</scalar>
       </property>
       <property dictRef="me:epsilon">
         <scalar>600.0</scalar>
       </property>
       <property dictRef="me:sigma">
         <scalar>6.2</scalar>
       </property>
     </propertyList>
   <me:energyTransferModel xsi:type="me:ExponentialDown">
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   </me:energyTransferModel>
   <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
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       <scalar units="kJ/mol">44.6</scalar>
     </property>
     <property dictRef="me:rotConsts">
         <array units="cm-1">
           0.096374
           0.062069
           0.042051
     </array>
     </property>
     <property dictRef="me:symmetryNumber">
       <scalar>1</scalar>
     </property>
```

```
<property dictRef="me:frequenciesScaleFactor">
  <scalar>0.974</scalar>
</property>
<property dictRef="me:vibFreqs">
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        141.6793
        213.4953
        230.9282
        291.3915
        319.4900
        352.7072
        374.1998
        447.1635
        539.7790
        594.6731
        670.3241
        701.8744
        841.8923
        877.6741
        905.2308
        954.8168
        957.5023
        1074.8320
        1112.0089
        1119.9504
        1132.9059
        1172.7942
        1175.4804
        1202.8281
        1290.4217
        1366.3255
        1383.6409
        1395.4798
        1405.7080
        1428.0240
        1487.1079
        1489.5283
        1495.1638
        1496.0774
        1679.8871
        2969.1820
        3067.9857
        3082.0739
        3117.8136
        3150.7411
        3162.4138
        3169.3479
        3180.5086
  </array>
</property>
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  <scalar units="amu">121.05008</scalar>
</property>
<property dictRef="me:spinMultiplicity">
  <scalar>2</scalar>
```

```
      </property>
      <property dictRef="me:imFreqs">
        <scalar units="cm-1">2201.4433</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
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    <propertyList>
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        <scalar units="kJ/mol">45.2</scalar>
      </property>
      <property dictRef="me:rotConsts">
          <array units="cm-1">
            0.095789
            0.056556
            0.050173
      </array>
      </property>
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      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
      <property dictRef="me:vibFreqs">
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            84.2451
            112.6676
            199.5594
            209.8030
            236.6937
            258.9526
            268.9934
            346.3859
            379.4615
            434.9340
            500.4151
            617.6594
            647.2881
            679.0320
            725.3785
            802.4669
            834.9314
            906.1239
            979.5671
            1019.7879
            1082.9857
            1115.6154
            1157.6697
            1174.8507
            1208.6457
            1369.8354
            1379.4129
            1407.5507
            1423.3364
```

```
                    1432.7445
                    1448.0008
                    1489.5734
                    1498.7654
                    1511.0392
                    1569.3983
                    3056.7067
                    3077.9940
                    3100.3124
                    3127.4219
                    3156.8733
                    3174.6967
                    3257.4759
                    3274.3736
                    3596.3200
        </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">121.05008</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:imFreqs">
        <scalar units="cm-1">506.8648</scalar>
      </property>
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
  </molecule>
  <molecule id="N2">
    <atom elementType="N2" />
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>3.9</scalar>
      </property>
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        <scalar units="amu">28.0</scalar>
      </property>
    </propertyList>
  </molecule>
</moleculeList>
<reactionList>
  <reaction id="Decomp">
    <reactant>
      <molecule ref="OQ2OOH" role="modelled" />
    </reactant>
    <product>
      <molecule ref="P1D" role="sink" />
    </product>
    <me:transitionState>
      <molecule ref="TS_D" role="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
```

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```
          <me:MCRCMethod name="SimpleRRKM"/>
      </reaction>
      <reaction id="H_Shift">
        <reactant>
          <molecule ref="OQ2OOH" role="modelled" />
        </reactant>
        <product>
          <molecule ref="P1H" role="sink" />
        </product>
        <me:transitionState>
          <molecule ref="TS_H" role="transitionState" />
        </me:transitionState>
        <me:tunneling name="Eckart"/>
        <me:MCRCMethod name="SimpleRRKM"/>
      </reaction>
    </reactionList>
    <me:conditions>
      <me:bathGas>N2</me:bathGas>
      <me:PTs>
        <me:PTpair units="Torr" P="760.0" T="233.0" />
        <me:PTpair units="Torr" P="760.0" T="243.0" />
        <me:PTpair units="Torr" P="760.0" T="253.0" />
        <me:PTpair units="Torr" P="760.0" T="263.0" />
        <me:PTpair units="Torr" P="760.0" T="273.0" />
        <me:PTpair units="Torr" P="760.0" T="283.0" />
        <me:PTpair units="Torr" P="760.0" T="293.0" />
        <me:PTpair units="Torr" P="760.0" T="298.15" />
        <me:PTpair units="Torr" P="760.0" T="303.0" />
        <me:PTpair units="Torr" P="760.0" T="313.0" />
        <me:PTpair units="Torr" P="760.0" T="323.0" />
        <me:PTpair units="Torr" P="760.0" T="333.0" />
        <me:PTpair units="Torr" P="760.0" T="343.0" />
      </me:PTs>
      <me:InitialPopulation>
        <me:molecule ref="OQ2OOH" population="1.0" />
      </me:InitialPopulation>
    </me:conditions>
    <me:modelParameters>
      <!--Specify grain size directly...-->
      <me:grainSize units="cm-1">50</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
      <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
    </me:modelParameters>
    <me:control>
      <me:printSpeciesProfile />
      <me:testRateConstants />
      <me:eigenvalues>10</me:eigenvalues>
    </me:control>
</me:mesmer>
```

******************************************** (CH3)2CHOC(OO)(CH3)2

```xml
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>DiPEyl + O2 With Internal Rotation</me:title>
  <moleculeList>
    <molecule id="O2" description="oxygen">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">1.597738</array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>2</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
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        </property>
        <property dictRef="me:MW">
          <scalar units="amu">32</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
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        </property>
      </propertyList>
      <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
    </molecule>
    <molecule id="R3" description="radical">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kJ/mol">0.0</scalar>
        </property>
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                0.1415550
                0.0537129
                0.0483179
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        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">
                86.4901
                98.6789
```

```
           171.9247
           180.8910
           184.2386
           223.2317
           252.1651
           322.1405
           357.6906
           406.7456
           411.9082
           491.5945
           515.9672
           797.1164
           864.8314
           941.9355
           949.2683
           954.9034
           958.3312
           979.5305
           1064.0958
           1097.0993
           1170.0681
           1181.4774
           1208.1809
           1306.2589
           1326.2200
           1375.8112
           1385.8788
           1403.3686
           1411.2191
           1420.3077
           1423.5346
           1471.0544
           1480.3459
           1481.4257
           1489.2193
           1493.3970
           1496.3505
           1503.9278
           1513.4972
           2990.0231
           2997.9465
           3040.7102
           3045.0835
           3056.0994
           3083.5170
           3088.6181
           3118.4564
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           3135.4372
           3149.5576
</array>
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<property dictRef="me:MW">
   <scalar units="amu">101.09664</scalar>
```

```xml
        </property>
        <property dictRef="me:spinMultiplicity">
          <scalar>2</scalar>
        </property>
        <property dictRef="me:epsilon">
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        </property>
        <property dictRef="me:sigma">
          <scalar>6.52</scalar>
        </property>
      </propertyList>
      <me:energyTransferModel xsi:type="me:ExponentialDown">
        <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
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      <me:DOSCMethod name="ClassicalRotors"/>
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    <molecule id="R300" description="ROO">
  <atomArray>
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   <atom id="a2" elementType="C" x3="1.424668" y3="0.063052" z3="-0.177781"/>
   <atom id="a3" elementType="H" x3="1.092297" y3="0.137972" z3="-1.215782"/>
   <atom id="a4" elementType="C" x3="2.350971" y3="-1.128455" z3="-0.010872"/>
   <atom id="a5" elementType="H" x3="1.860906" y3="-2.056709" z3="-0.301772"/>
   <atom id="a6" elementType="H" x3="3.245367" y3="-1.004021" z3="-0.621506"/>
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   <atom id="a8" elementType="C" x3="2.082460" y3="1.369772" z3="0.222076"/>
   <atom id="a9" elementType="H" x3="2.969118" y3="1.553897" z3="-0.384305"/>
   <atom id="a10" elementType="H" x3="1.384022" y3="2.194867" z3="0.094037"/>
   <atom id="a11" elementType="H" x3="2.379758" y3="1.326518" z3="1.270295"/>
   <atom id="a12" elementType="C" x3="-0.941448" y3="-1.663322" z3="-0.754608"/>
   <atom id="a13" elementType="H" x3="-0.701774" y3="-2.513999" z3="-0.119352"/>
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   <atom id="a15" elementType="H" x3="-0.214682" y3="-1.606279" z3="-1.562715"/>
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   <atom id="a17" elementType="H" x3="-1.751128" y3="-1.187937" z3="1.890776"/>
   <atom id="a18" elementType="H" x3="-1.942824" y3="0.564027" z3="1.692502"/>
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   <atom id="a20" elementType="C" x3="-0.929095" y3="-0.401872" z3="0.088328"/>
   <atom id="a21" elementType="O" x3="-1.275373" y3="0.653792" z3="-0.895985"/>
   <atom id="a22" elementType="O" spinMultiplicity="2" x3="-1.257244"
  y3="1.839110" z3="-0.379715"/>
  </atomArray>
  <bondArray>
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   <bond atomRefs2="a3 a2" order="1"/>
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   <bond id="b1" atomRefs2="a21 a20" order="1"/>
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   <bond atomRefs2="a2 a8" order="1"/>
   <bond atomRefs2="a2 a1" order="1"/>
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```xml
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<bond atomRefs2="a20 a1" order="1"/>
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<bond atomRefs2="a19 a16" order="1"/>
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      </property>
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            0.0438450
            0.0345556
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      </property>
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        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
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            90.6073
            188.8728
            196.9884
            239.5326
            250.5359
            283.9924
            298.6257
            310.6634
            329.4303
            362.9969
            419.6144
            468.9534
            479.0846
            552.2562
            617.5498
            762.8031
            829.8768
            884.6818
            931.8872
            940.7642
            948.3883
            956.4169
            1018.4141
            1079.2376
            1152.9246
            1172.1848
            1183.9621
```

```
           1211.4731
           1289.6955
           1292.4602
           1320.0534
           1367.9276
           1400.8882
           1405.5711
           1410.3789
           1421.2022
           1426.0865
           1480.3554
           1486.2736
           1486.5723
           1490.0793
           1495.8023
           1503.3835
           1511.6834
           1514.9257
           3045.8355
           3049.8577
           3068.0655
           3072.7016
           3075.377
           3119.6276
           3127.8539
           3130.8007
           3138.6629
           3151.8803
           3155.5595
           3162.3001
           3166.2899
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     </property>
    <property dictRef="me:epsilon">
      <scalar>560.0</scalar>
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    <property dictRef="me:sigma">
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    </property>
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   <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
</me:energyTransferModel>
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   <me:bondRef>b1</me:bondRef>
   <me:HinderedRotorPotential format="numerical" units="kJ/mol"
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        162.816
        183.4619
        193.4954
        208.234
        234.5153
        270.076
        280.0639
        333.8413
        347.7769
        375.2482
        378.224
        403.9147
        429.0883
        460.6499
        578.154
        624.2887
        783.8024
        846.1125
        913.3156
        945.404
        946.3728
        969.5266
        983.4419
        1024.0631
        1057.7673
        1070.3767
        1104.2996
        1206.622
        1257.3368
        1273.3994
        1305.676
        1330.3895
        1402.9649
        1412.299
        1416.0844
        1422.1637
        1458.9989
        1472.2098
        1479.5605
        1482.9036
        1490.6733
        1493.2603
        1499.2304
        1509.8329
        1517.0291
        2994.6136
        2999.0171
        3076.7982
```

```
                    3082.3902
                    3095.878
                    3100.8339
                    3136.7494
                    3148.5424
                    3153.9295
                    3160.4946
                    3171.9447
                    3180.1157
                    3706.2686
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    </property>
    <property dictRef="me:epsilon">
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    </property>
    <property dictRef="me:sigma">
      <scalar>6.82</scalar>
    </property>
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    <me:deltaEDown units="cm-1">250.0</me:deltaEDown>
  </me:energyTransferModel>
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    </property>
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            103.1025
            159.5862
            182.4606
            215.5994
            252.6128
```

```
                         259.7257
                         283.3073
                         323.4348
                         333.621
                         377.8351
                         406.4435
                         456.4242
                         515.2567
                         541.99
                         562.5926
                         639.7869
                         804.7665
                         854.1153
                         897.8409
                         937.1375
                         944.1242
                         961.3675
                         973.054
                         1022.6241
                         1057.3004
                         1089.3655
                         1134.8054
                         1160.8336
                         1206.2593
                         1256.3482
                         1265.9738
                         1273.2143
                         1303.7347
                         1397.2419
                         1409.2462
                         1412.1341
                         1424.4582
                         1471.6214
                         1476.4269
                         1481.7016
                         1487.7894
                         1494.4412
                         1495.1226
                         1500.0039
                         1518.7257
                         1659.2084
                         3032.5429
                         3038.5228
                         3073.8402
                         3082.0134
                         3108.4808
                         3115.1705
                         3139.5173
                         3148.5753
                         3154.2683
                         3164.6502
                         3172.5734
                         3173.0258
</array>
</property>
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            </property>
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0.070631983
0.054923849
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            </property>
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105.0616
155.0602
226.9255
314.251
372.3583
424.2656
456.0055
528.59
682.9059
963.6882
981.4374
1018.727
1106.512
1134.017
1184.574
1234.109
1289.467
1314.044
1330.885
1411.263
1439.189
1462.25
1490.188
1517.613
```

```
3090.145
3096.316
3170.854
3180.728
3779.973
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        <property dictRef="me:sigma">
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  </moleculeList>
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      <reactant>
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      <reactant>
        <molecule ref="O2" role="excessReactant" />
      </reactant>
      <product>
        <molecule ref="R3OO" role="modelled" />
      </product>
      <me:MCRCMethod xsi:type="me:MesmerILT">
        <me:preExponential units="cm3molecule-1s-1">6.00e-12</me:preExponential>
        <me:activationEnergy units="kJ/mol">0.0</me:activationEnergy>
        <me:TInfinity>298.0</me:TInfinity>
        <me:nInfinity>0.00000000001</me:nInfinity>
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      <me:excessReactantConc>4.67E18</me:excessReactantConc>
    </reaction>
      <reaction id="H_shift" reversible="true">
      <reactant>
        <molecule ref="R3OO" role="modelled" />
      </reactant>
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        <molecule ref="Q3OOH" role="modelled" />
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```xml
        </product>
        <me:transitionState>
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        <me:tunneling name="Eckart"/>
        <me:MCRCMethod name="SimpleRRKM"/>
      </reaction>
      <reaction id="Q3OOH_O2">
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        <reactant>
          <molecule ref="O2" role="excessReactant" />
        </reactant>
        <product>
          <molecule ref="OOQ3OOH" role="sink" />
        </product>
        <me:MCRCMethod name="SimpleBimolecularSink"/>

<me:BimolecularLossRateCoefficient>6.00e-12</me:BimolecularLossRateCoefficient>
        <me:excessReactantConc>4.67E18</me:excessReactantConc>
      </reaction>
    </reactionList>
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      <me:InitialPopulation>
        <me:molecule ref="R3" population="1.0" />
      </me:InitialPopulation>
    </me:conditions>
    <me:modelParameters>
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      <me:grainSize units="cm-1">50</me:grainSize>
      <!--...or by the total number of grains
          <me:numberOfGrains> 500 </me:numberOfGrains>-->
      <!--Specify increased energy range
          <me:maxTemperature>6000</me:maxTemperature>-->
      <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
      <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
    </me:modelParameters>
    <me:control>
      <me:printSpeciesProfile />
      <me:testRateConstants />
```

```
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
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*************************************** (CH3)2C(O)OC(OOH)(CH3)2

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>(CH3)2C(OOH)OC(O)(CH3)2 H-Shift and CH3-Elimination</me:title>
  <moleculeList>
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        </property>
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        </property>
        <property dictRef="me:frequenciesScaleFactor">
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                135.8256
                176.2905
                206.025
                219.1042
                224.8614
                240.6054
                285.9782
                302.3917
                314.6968
                332.5812
                363.1922
                377.8464
                389.3541
                416.3332
                477.067
                525.7727
                548.148
                591.6906
                653.1212
                780.7237
```

```
          831.7658
          905.7679
          914.392
          936.5639
          950.9015
          955.2263
          963.1731
          1020.2948
          1053.7233
          1067.2567
          1139.1175
          1159.9747
          1185.6082
          1250.4626
          1255.2175
          1295.5583
          1373.7433
          1400.3066
          1410.0955
          1427.1843
          1471.6906
          1480.2166
          1482.7619
          1483.8332
          1488.2192
          1494.3078
          1500.3363
          1511.6734
          1524.4625
          3066.29
          3074.2026
          3075.3463
          3077.9137
          3147.9851
          3153.7409
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          3167.6643
          3170.8581
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            0.032292
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             192.8250
             207.7498
             225.9635
             244.9940
             256.0510
             275.4453
             288.9887
             322.5749
             333.2254
             354.8107
             384.3943
             448.7002
             497.2777
             561.5120
             568.1677
             640.3546
             671.4234
             717.0549
             770.8737
             800.3821
             855.5345
             912.0550
             957.5892
             987.2852
            1024.4013
            1032.8610
            1051.3763
```

```
                1082.6801
                1134.6818
                1170.4134
                1250.1590
                1261.7971
                1301.8139
                1403.7068
                1412.7549
                1423.3953
                1428.0906
                1451.6050
                1479.1186
                1482.4770
                1485.8371
                1486.6848
                1496.9356
                1503.2841
                1512.8343
                1552.0585
                3067.3136
                3077.1435
                3078.3804
                3106.3169
                3149.5760
                3152.6695
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                3188.4256
                3258.4440
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      <property dictRef="me:spinMultiplicity">
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       253.5256
       278.2446
       302.3067
       328.9242
       352.7037
       369.7639
       378.8114
       383.1079
       445.9523
       479.7825
       526.0657
       573.3028
       643.0115
       654.1526
       783.7819
       830.2792
       841.7876
       905.1108
       926.8131
       938.3111
       946.3024
       980.5661
      1008.9715
      1020.7123
      1068.5814
      1139.3183
      1163.1743
      1193.7202
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      1380.8836
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      1408.6675
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      1480.0594
      1484.6419
      1488.3278
      1496.4764
```

```
                    1500.3548
                    1514.1960
                    1521.3586
                    1638.6132
                    3070.0621
                    3070.5125
                    3074.2551
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                    3149.2114
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    </property>
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    </property>
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          176.2905
          206.025
          219.1042
          224.8614
```

240.6054
285.9782
302.3917
314.6968
332.5812
363.1922
377.8464
389.3541
416.3332
477.067
525.7727
548.148
591.6906
653.1212
780.7237
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905.7679
914.392
936.5639
950.9015
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1159.9747
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1427.1843
1471.6906
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1482.7619
1483.8332
1488.2192
1494.3078
1500.3363
1511.6734
1524.4625
3066.29
3074.2026
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3077.9137
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3170.8581
3175.694
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        </property>
        <property dictRef="me:frequenciesScaleFactor">
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        </property>
        <property dictRef="me:vibFreqs">
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                135.8256
                176.2905
                206.025
                219.1042
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                240.6054
                285.9782
                302.3917
                314.6968
                332.5812
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                377.8464
                389.3541
                416.3332
```

```
          477.067
          525.7727
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          936.5639
          950.9015
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          1020.2948
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          1067.2567
          1139.1175
          1159.9747
          1185.6082
          1250.4626
          1255.2175
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          1494.3078
          1500.3363
          1511.6734
          1524.4625
          3066.29
          3074.2026
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    <atom elementType="N2" />
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      </property>
      <property dictRef="me:sigma">
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</moleculeList>
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      <molecule ref="OQ3OOH" role="modelled" />
    </reactant>
    <product>
      <molecule ref="P1D" role="sink" />
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    <me:transitionState>
      <molecule ref="TS_D" role="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
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<me:conditions>
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    <me:InitialPopulation>
      <me:molecule ref="OQ3OOH" population="1.0" />
    </me:InitialPopulation>
  </me:conditions>
  <me:modelParameters>
    <!--Specify grain size directly...-->
    <me:grainSize units="cm-1">50</me:grainSize>
    <!--...or by the total number of grains
        <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
        <me:maxTemperature>6000</me:maxTemperature>-->
    <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
    <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
  </me:modelParameters>
  <me:control>
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
```

******************************************** CH3CH2OCH(O)CH3

```
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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen' ?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>CH3CH2OCH(O)CH3 Unimolecular Reactions</me:title>
  <moleculeList>
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        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">
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              0.0669082
              0.0572131
          </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
```

```
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           125.6650
           191.3618
           218.9428
           265.0045
           342.7207
           406.0155
           473.9907
           614.7120
           819.6394
           866.4358
           918.8325
           966.0182
          1028.1013
          1095.7952
          1120.8356
          1190.9983
          1197.8317
          1224.0272
          1236.8164
          1310.5645
          1334.4684
          1397.2853
          1409.5260
          1454.8839
          1496.3648
          1500.1501
          1508.3999
          1518.1914
          1545.7755
          2897.0400
          3020.6213
          3081.8244
          3093.4255
          3094.2311
          3166.7333
          3171.9471
          3186.9942
          3200.0420
    </array>
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<property dictRef="me:spinMultiplicity">
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</property>
<property dictRef="me:epsilon">
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</property>
<property dictRef="me:sigma">
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```xml
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            0.2667820
            0.0669082
            0.0572131
      </array>
      </property>
      <property dictRef="me:symmetryNumber">
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            191.3618
            218.9428
            265.0045
            342.7207
            406.0155
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            614.7120
            819.6394
            866.4358
            918.8325
            966.0182
            1028.1013
            1095.7952
            1120.8356
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            1197.8317
            1224.0272
            1236.8164
            1310.5645
            1334.4684
            1397.2853
            1409.5260
            1454.8839
            1496.3648
            1500.1501
            1508.3999
            1518.1914
```

```
                1545.7755
                2897.0400
                3020.6213
                3081.8244
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                3166.7333
                3171.9471
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      </property>
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            0.0572131
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      </property>
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            191.3618
            218.9428
            265.0045
            342.7207
```

```
                  406.0155
                  473.9907
                  614.7120
                  819.6394
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                  918.8325
                  966.0182
                  1028.1013
                  1095.7952
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                  1190.9983
                  1197.8317
                  1224.0272
                  1236.8164
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                  1397.2853
                  1409.5260
                  1454.8839
                  1496.3648
                  1500.1501
                  1508.3999
                  1518.1914
                  1545.7755
                  2897.0400
                  3020.6213
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                  3093.4255
                  3094.2311
                  3166.7333
                  3171.9471
                  3186.9942
                  3200.0420
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        55.9043
        125.6650
        191.3618
        218.9428
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        406.0155
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        819.6394
        866.4358
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        966.0182
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        1508.3999
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        2897.0400
        3020.6213
        3081.8244
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        3166.7333
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```

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  </me:energyTransferModel>
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          0.0669082
          0.0572131
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    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
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          819.6394
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          966.0182
          1028.1013
          1095.7952
          1120.8356
```

```
                    1190.9983
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                    1236.8164
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                    1397.2853
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        <scalar units="kJ/mol">28.8</scalar>
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      <property dictRef="me:rotConsts">
          <array units="cm-1">
            0.2158646
            0.0701244
            0.0613086
      </array>
      </property>
      <property dictRef="me:symmetryNumber">
```

```
    <scalar>1</scalar>
</property>
<property dictRef="me:frequenciesScaleFactor">
    <scalar>0.974</scalar>
</property>
<property dictRef="me:vibFreqs">
    <array units="cm-1">
            80.4989
            135.9771
            156.1413
            227.0309
            251.7943
            270.2083
            389.0961
            440.6791
            671.7967
            675.6480
            793.1712
            815.6592
            878.3779
            955.6753
            1064.1102
            1095.8978
            1143.1751
            1185.1041
            1199.3712
            1313.3665
            1354.6523
            1402.0203
            1426.5096
            1436.2436
            1442.9997
            1491.2644
            1505.4518
            1530.9940
            1570.3997
            3031.5122
            3062.2460
            3071.5581
            3092.3545
            3110.6660
            3135.6353
            3152.0913
            3248.9503
            3260.3795
    </array>
</property>
<property dictRef="me:MW">
    <scalar units="amu">89.06025</scalar>
</property>
<property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
</property>
<property dictRef="me:imFreqs">
    <scalar units="cm-1">571.7592</scalar>
</property>
```

```
    </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
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    <propertyList>
        <property dictRef="me:ZPE">
            <scalar units="kJ/mol">39.2</scalar>
        </property>
        <property dictRef="me:rotConsts">
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                0.2683776
                0.0687436
                0.0576338
        </array>
        </property>
        <property dictRef="me:symmetryNumber">
            <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
            <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
            <array units="cm-1">
                88.1355
                143.2249
                191.0211
                204.6218
                278.5567
                375.3742
                423.1791
                534.9778
                606.2305
                666.3969
                696.0305
                814.0074
                884.2501
                970.6192
                1025.6887
                1075.2071
                1117.8869
                1158.6199
                1188.9142
                1271.7352
                1312.5949
                1395.4053
                1406.2907
                1438.5339
                1478.2479
                1486.7360
                1498.6143
                1504.3550
                1527.9876
                1658.8648
                3064.5460
                3069.1508
                3071.5557
```

```
                    3111.8382
                    3149.5571
                    3151.6337
                    3152.8472
                    3189.7142
        </array>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">89.06025</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
          <scalar>2</scalar>
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        <property dictRef="me:imFreqs">
          <scalar units="cm-1">1113.9666</scalar>
        </property>
      </propertyList>
    <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>
</molecule>
<molecule id="TS3_CO_Break">
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          <scalar units="kJ/mol">78.2</scalar>
        </property>
        <property dictRef="me:rotConsts">
            <array units="cm-1">
              0.2618818
              0.0626148
              0.0540039
        </array>
        </property>
        <property dictRef="me:symmetryNumber">
          <scalar>1</scalar>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
          <scalar>0.974</scalar>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">
              57.0692
              111.3627
              157.7522
              203.7515
              283.1068
              309.661
              333.1093
              459.1481
              519.055
              816.5497
              885.566
              909.8426
              970.8621
              1012.0191
              1111.2411
              1137.7094
              1163.7767
```

```
                    1179.3438
                    1290.1841
                    1361.9524
                    1379.552
                    1398.665
                    1399.6102
                    1468.9907
                    1481.2331
                    1492.9223
                    1505.2013
                    1530.6407
                    1575.0424
                    3018.6194
                    3049.803
                    3067.5355
                    3069.8208
                    3104.2884
                    3144.7796
                    3151.1296
                    3157.6907
                    3173.0741
      </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">89.06025</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:imFreqs">
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    </propertyList>
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</molecule>
<molecule id="TS4_H_Shift">
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        <scalar units="kJ/mol">58.8</scalar>
      </property>
      <property dictRef="me:rotConsts">
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            0.2320350
            0.0918939
            0.0716145
      </array>
      </property>
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        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>0.974</scalar>
      </property>
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        <array units="cm-1">
            128.7383
```

```
                216.3656
                282.2269
                315.4198
                405.9988
                482.9925
                533.6941
                607.5925
                731.6792
                860.7941
                869.1666
                921.0216
                961.8909
               1089.9562
               1120.3486
               1132.7786
               1138.9471
               1176.4197
               1191.3359
               1277.1777
               1303.5677
               1374.3155
               1384.5320
               1397.7548
               1423.8545
               1460.6730
               1484.5011
               1493.4576
               1503.8118
               1573.3953
               3009.8452
               3030.8486
               3070.2889
               3102.0749
               3115.1884
               3156.1156
               3162.8423
               3199.8431
      </array>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">89.06025</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
      </property>
      <property dictRef="me:imFreqs">
        <scalar units="cm-1">1579.1212</scalar>
      </property>
    </propertyList>
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</molecule>
<molecule id="N2">
    <atom elementType="N2"/>
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
```

```
        </property>
        <property dictRef="me:sigma">
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        </property>
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      </propertyList>
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  </moleculeList>
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      <reactant>
        <molecule ref="CH3CH2OCHOCH3" role="modelled" />
      </reactant>
      <product>
        <molecule ref="P1" role="sink" />
      </product>
      <me:transitionState>
        <molecule ref="TS1_De_CH3" role="transitionState" />
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
    <reaction id="R2_De_H">
      <reactant>
        <molecule ref="CH3CH2OCHOCH3" role="modelled" />
      </reactant>
      <product>
        <molecule ref="P2" role="sink" />
      </product>
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        <molecule ref="TS2_De_H" role="transitionState" />
      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
    <reaction id="R3_CO_Break">
      <reactant>
        <molecule ref="CH3CH2OCHOCH3" role="modelled" />
      </reactant>
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        <molecule ref="P3" role="sink" />
      </product>
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      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
    <reaction id="R4_H_Shift">
      <reactant>
        <molecule ref="CH3CH2OCHOCH3" role="modelled" />
      </reactant>
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        <molecule ref="P4" role="sink" />
```

```xml
      </product>
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      </me:transitionState>
      <me:tunneling name="Eckart"/>
      <me:MCRCMethod name="SimpleRRKM"/>
    </reaction>
  </reactionList>
  <me:conditions>
    <me:bathGas>N2</me:bathGas>
    <me:PTs>
      <me:PTpair units="Torr" P="760.0" T="233.0" />
      <me:PTpair units="Torr" P="760.0" T="243.0" />
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      <me:PTpair units="Torr" P="760.0" T="323.0" />
      <me:PTpair units="Torr" P="760.0" T="333.0" />
    </me:PTs>
    <me:InitialPopulation>
      <me:molecule ref="CH3CH2OCHOCH3" population="1.0" />
    </me:InitialPopulation>
  </me:conditions>
  <me:modelParameters>
    <!--Specify grain size directly...-->
    <me:grainSize units="cm-1">50</me:grainSize>
    <!--...or by the total number of grains
        <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
        <me:maxTemperature>6000</me:maxTemperature>-->
    <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
    <me:automaticallySetMaxEne>1.0e-09</me:automaticallySetMaxEne>
  </me:modelParameters>
  <me:control>
    <me:printSpeciesProfile />
    <me:testRateConstants />
    <me:eigenvalues>10</me:eigenvalues>
  </me:control>
</me:mesmer>
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