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

Exploring the features on the OH + SO_2 potential energy surface using theory and testing its accuracy by comparison to experimental data

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Supporting Information

1. Comparison of modelled and measured rate coefficients for k_1

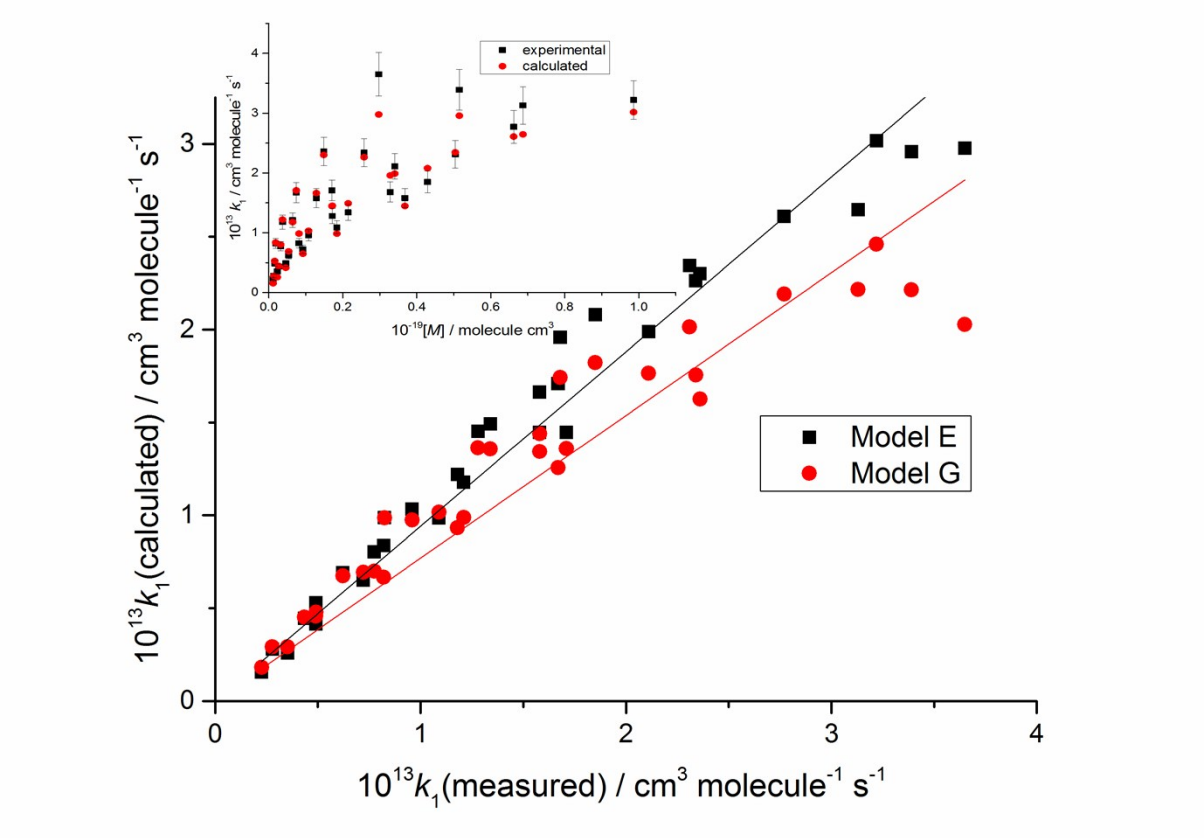

Figure S1. Plots from the MESMER analysis of literature data, k_1(measured), against the calculated values from Models E(slope = 0.94) slope and F(slope = 0.77). A slope equal to 1 would be a perfect fit. The inset is the Model E fit to the literature data versus bath gas concentration.

2. Troe parameterisation for $k_1(p,T)$ for OH + SO_2

$k_0(T) = A_0 \times (T/298)^n$ cm^6 molecule^{-2} s^{-1}

$k^\infty(T) = A_{inf} \times (T/298)^m$ cm^3 molecule^{-1} s^{-1}

Broadening parameters based on Troe and Ushakov (Troe, J. and V. G. Ushakov (2014). "Representation of "Broad" Falloff Curves for Dissociation and Recombination Reactions." Z. Phys. Chem. (Muenchen, Ger.) **228**(1): 1-10.)

For $x = k_0[M]/k_\infty$,

Troe and Ushakov give $F(x) = (1 + \frac{x}{x_0})/[1 + (\frac{x}{x_0})^n]^{1/n}$

with $n = \left[\frac{ln2}{\ln\left(\frac{2}{F_{cent}}\right)}\right][1 - b + b\left(\frac{x}{x_0}\right)^q]$

where $q = (F_{cent} - 1)/ln(\frac{F_{cent}}{10})$, the parameter x_0 is in the range 0.9 – 1.1 and b is in the range 0.1 – 0.25.

Parameterized form of $F_{cent}(T) = F_{cent}A \times \exp(-F_{cent}B \times T) + F_{cent}C$

Troe parameters for nitrogen buffer gas

$k_{1,N2}(p,T)$:

$k^\infty(T) = 5.99\times10^{-13} \times (T/298)^{-0.12}$ cm^3 molecule^{-1} s^{-1}

$k_0(T) = 1.41\times10^{-30} \times (T/298)^{-3.95}$ cm^6 molecule^{-2} s^{-1}

$x_0 = 0.980$

$b = 0.215$

$F_{cent} = 0.394 \times \exp(-0.0001444 \times T) - 0.00$

$k_{1,He}(p,T)$:

$k^\infty(T) = 6.00\times10^{-13} \times (T/298)^{-0.12}$ cm^3 molecule^{-1} s^{-1}

$k_0(T) = 5.418\times10^{-31} \times (T/298)^{-2.62}$ cm^6 molecule^{-2} s^{-1}

$x_0 = 0.958$

$b = 0.212$

$F_{cent} = 0.418 \times \exp(-0.000494 \times T) - 0.00$

$\boldsymbol{k_{1,Ar}(p,T)}$:

$k^{\infty}(T) = 5.99\times10^{-13} \times (T/298)^{-0.12}$ cm^3 molecule^{-1} s^{-1}

$k_0(T) = 1.09\times10^{-30} \times (T/298)^{-3.87}$ cm^6 molecule^{-2} s^{-1}

$x_0 = 0.974$

$b = 0.212$

$F_{cent} = 0.369 \times \exp(-0.0000328 \times T) - 0.00$

3. Input parameters for the MESMER master equation analysis

OH + SO_2 Mesmer xml input with vdW complex

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  1.19470688E-01 -5.00494566E-01  1.36258087E-01 -1.06523965E-02 -3.20275776E-02
  1.05965950E-02  4.84598715E-03 -3.25219967E-03  1.90938177E-04 -1.26241075E-01
  5.46692286E-01 -4.82547398E-02  1.75354721E-01 -1.28093155E-01  4.28312381E-03
 -8.42848532E-03  1.93044077E-02  8.86856069E-04  1.89831453E-03 -1.07575073E-03
  3.92329974E-02 -1.53689197E-01  8.33951433E-02 -4.36463746E-01  2.08105729E-01
  1.35142945E-01 -3.87729443E-02  1.37789608E-02  8.93873807E-03 -9.31398318E-04
 -6.96445161E-03  3.37028346E-03 -1.40832178E-03  1.25767960E-02  3.85176258E-03
  4.77576410E-01  2.10407492E-01 -1.84410369E-01 -7.38409610E-02 -1.03426873E-02
  1.74687219E-02  7.53965849E-03 -2.31998896E-03 -1.59776750E-03  9.29837920E-06
  2.97522184E-02 -1.09179432E-02 -1.51353527E-02 -2.27497034E-01  1.79457358E-01
  1.72337709E-01 -9.36614404E-02 -1.33757796E-01 -5.34915563E-03  6.00947031E-03
  1.60681192E-02 -2.36250199E-03 -4.18963521E-04  1.37826625E-03 -1.33223218E-02
  6.64357673E-03  2.64693548E-02 -1.51303729E-01  8.14273569E-02  8.98420555E-02
</matrix>
</property>
<property dictRef = "me:rotConsts">
<array units="cm-1">0.314502 0.303562 0.164708 </array>
</property>
 <property dictRef="me:MW">
        <scalar units="amu">81</scalar>
       </property>
       <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
       </property>
                              <property dictRef="me:epsilon">
        <scalar>473.17</scalar>
       </property>
       <property dictRef="me:sigma">
        <scalar>5.09</scalar>
```

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      </property>
    </propertyList>

    <me:DOSCMethod>Classical rotors</me:DOSCMethod>
                <me:energyTransferModel xsi:type="me:ExponentialDown">

                 <me:deltaEDown  bathGas="He" units="cm-1" lower="100" upper="250" stepsize="10">120</me:deltaEDown>
                          <!-- <me:deltaEDownTExponent bathGas="He" referenceTemperature="298" lower="0.99" upper="1.01"
stepsize="0.005" >1.00</me:deltaEDownTExponent> -->
                 <me:deltaEDownTExponent bathGas="He">1.00</me:deltaEDownTExponent>

                <me:deltaEDown  bathGas="Ar" units="cm-1" lower="100" upper="350" stepsize="10">232</me:deltaEDown>
                 <me:deltaEDownTExponent bathGas="Ar">0.5</me:deltaEDownTExponent>
      </me:energyTransferModel>

<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
 <me:bondRef>b1</me:bondRef>
<me:HinderedRotorPotential format="numerical" units="Hartree" expansionSize="10" UseSineTerms="yes" scale="1">
<me:PotentialPoint angle="-25.741" potential="-624.425740"/>
  <me:PotentialPoint angle="-10.741" potential="-624.425420"/>
  <me:PotentialPoint angle="4.259" potential="-624.424550"/>
  <me:PotentialPoint angle="19.259" potential="-624.423330"/>
  <me:PotentialPoint angle="34.259" potential="-624.422060"/>
  <me:PotentialPoint angle="49.259" potential="-624.421060"/>
  <me:PotentialPoint angle="64.259" potential="-624.420620"/>
  <me:PotentialPoint angle="79.259" potential="-624.420870"/>
  <me:PotentialPoint angle="94.259" potential="-624.421750"/>
  <me:PotentialPoint angle="109.259" potential="-624.422970"/>
  <me:PotentialPoint angle="124.259" potential="-624.424230"/>
  <me:PotentialPoint angle="139.259" potential="-624.425230"/>
  <me:PotentialPoint angle="154.259" potential="-624.425750"/>
  <me:PotentialPoint angle="169.259" potential="-624.425590"/>
  <me:PotentialPoint angle="-175.741" potential="-624.424770"/>
  <me:PotentialPoint angle="-160.741" potential="-624.423410"/>
  <me:PotentialPoint angle="-145.741" potential="-624.421850"/>
  <me:PotentialPoint angle="-130.741" potential="-624.420550"/>
  <me:PotentialPoint angle="-115.741" potential="-624.419960"/>
  <me:PotentialPoint angle="-100.741" potential="-624.420330"/>
  <me:PotentialPoint angle="-85.741" potential="-624.421480"/>
  <me:PotentialPoint angle="-70.741" potential="-624.423000"/>
  <me:PotentialPoint angle="-55.741" potential="-624.424440"/>
  <me:PotentialPoint angle="-40.741" potential="-624.425420"/>
  <me:PotentialPoint angle="-25.741" potential="-624.425770"/>
 </me:HinderedRotorPotential>
</me:ExtraDOSCMethod>
</molecule>

 <molecule id="He">
    <atom elementType="He"/>
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>10.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>2.55</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar>4.0</scalar>
      </property>
    </propertyList>
  </molecule>

              <molecule id="N2">
    <atom elementType="N2"/>
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>3.90</scalar>
      </property>
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```
      <property dictRef="me:MW">
       <scalar units="amu">28.0</scalar>
      </property>
     </propertyList>
    </molecule>

              <molecule id="Ar">
     <atom elementType="Ar"/>
     <propertyList>
      <property dictRef="me:epsilon">
       <scalar>114</scalar>
      </property>
      <property dictRef="me:sigma">
       <scalar>3.47</scalar>
      </property>
      <property dictRef="me:MW">
       <scalar units="amu">40.0</scalar>
      </property>
     </propertyList>
    </molecule>

</moleculeList>


 <reactionList>
  <reaction id="R1">
     <reactant>
      <molecule ref="OH" me:type="deficientReactant"/>
     </reactant>
     <reactant>
      <molecule ref="SO2" me:type="excessReactant"/>
     </reactant>
     <product>
      <molecule ref="PRE_COMPLEX" me:type="modelled"/>
     </product>
     <me:excessReactantConc>1e15</me:excessReactantConc>

     <me:MCRCMethod>MesmerILT</me:MCRCMethod>
     <me:preExponential>1.3e-10</me:preExponential>
     <!-- <me:preExponential lower="1E-14" upper="5.0E-10" stepsize="1.0E-14">1.36e-10</me:preExponential> -->
               <!--  <me:activationEnergy units="kJ/mol" lower="0.01" upper="2.0" stepsize="0.1">0.97</me:activationEnergy> -->
     <me:activationEnergy>0.0</me:activationEnergy>
      <me:TInfinity>298.0</me:TInfinity>
     <me:nInfinity>0.5</me:nInfinity>
               </reaction>

              <reaction id="R2">
     <reactant>
      <molecule ref="PRE_COMPLEX" role="modelled" />
     </reactant>
     <product>
      <molecule ref="HOSO2" role="modelled" />
     </product>
     <me:transitionState>
      <molecule ref="TS_1" role="transitionState" />
     </me:transitionState>
                 <me:tunneling name="Eckart"/>
     <me:MCRCMethod name="SimpleRRKM"/>
   </reaction>

 </reactionList>

  <me:conditions>
   <me:bathGas>He</me:bathGas>

               <me:PTs>
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                 <me:PTpair units="Torr" P="100.3" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="17">168</me:experimentalRate> </me:PTpair>
     <me:PTpair units="Torr" P="209.9" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="31">313</me:experimentalRate> </me:PTpair>
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```
    <me:PTpair units="Torr" P="52.5" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="13">128</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="24.9" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="83">82.5</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="52.2" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="17">171</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="301.2" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="63.128">322</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="104" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="21">211</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="154" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="23">231</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="202.2" T="295" precision="d"> <me:experimentalRate ref1="OH" ref2="OH"
error="28">277</me:experimentalRate> </me:PTpair>

                <!--BLITZ2003-->
                 <me:PTpair units="Torr" P="506" T="523" precision="d"> <me:experimentalRate ref1="HOSO2" ref2="HOSO2"
error="64">316</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="508" T="543" precision="d"> <me:experimentalRate ref1="HOSO2" ref2="HOSO2"
error="74">371</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="509" T="563" precision="d"> <me:experimentalRate ref1="HOSO2" ref2="HOSO2"
error="135">672</me:experimentalRate> </me:PTpair>
    <me:PTpair units="Torr" P="504" T="583" precision="d"> <me:experimentalRate ref1="HOSO2" ref2="HOSO2"
error="170">852</me:experimentalRate> </me:PTpair>

                <!--WINE-->
                  <me:PTpair units="Torr" P="5" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="4.9">49.1</me:experimentalRate>    </me:PTpair>
                <me:PTpair units="Torr" P="10" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="7.8">77.5</me:experimentalRate>   </me:PTpair>
                <me:PTpair units="Torr" P="20" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="12.1">121</me:experimentalRate>   </me:PTpair>
     <me:PTpair units="Torr" P="40" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH" ref2="OH"
error="15.8">158</me:experimentalRate>  </me:PTpair>
                <me:PTpair units="Torr" P="80" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="23.4">234</me:experimentalRate>  </me:PTpair>
     <me:PTpair units="Torr" P="160" T="300" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="33.9">339</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="5" T="260" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="8.21">82.1</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="5" T="360" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="5">27.9</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="5" T="420" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="5">22.6</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="10" T="260" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="11.8">118</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="10" T="360" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="5">43.5</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="10" T="420" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="5">35.3</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="20" T="260" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="17">167</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="20" T="360" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="6.2">62.2</me:experimentalRate> </me:PTpair>
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ref2="OH" error="5">49.0</me:experimentalRate> </me:PTpair>
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ref2="OH" error="24">236</me:experimentalRate> </me:PTpair>
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ref2="OH" error="10">95.9</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="40" T="420" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="7.2">72.2</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="80" T="260" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="37">365</me:experimentalRate> </me:PTpair>
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ref2="OH" error="13.4">134</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="80" T="420" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="11">109</me:experimentalRate> </me:PTpair>
                <me:PTpair units="Torr" P="160" T="360" precision="d"> <me:bathGas>Ar</me:bathGas> <me:experimentalRate ref1="OH"
ref2="OH" error="19">185</me:experimentalRate> </me:PTpair>
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```
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ref2="OH" error="16">158</me:experimentalRate> </me:PTpair>

                            </me:PTs>
 </me:conditions>
 <me:modelParameters>
  <!--Specify grain size directly...-->
  <me:grainSize units="cm-1">50</me:grainSize>
  <me:energyAboveTheTopHill>25.</me:energyAboveTheTopHill>
 </me:modelParameters>

  <me:control>

     <me:calcMethod>marquardt</me:calcMethod>
                        <me:MarquardtIterations>5</me:MarquardtIterations>
                        <me:MarquardtTolerance>1e-6</me:MarquardtTolerance>
                        <me:MarquardtDerivDelta>0.025</me:MarquardtDerivDelta>
              <me:printGrainBoltzmann />
              <me:printGrainedSpeciesProfile />
   <me:printSpeciesProfile/>
   <me:testRateConstants/>
   <me:eigenvalues>5</me:eigenvalues>
 </me:control>


 <!--  <me:control>
  <me:calcMethod units="kJ/mol" xsi:type="me:ThermodynamicTable">
    <me:Tmin>0</me:Tmin>
    <me:Tmid>500</me:Tmid>
    <me:Tmax>1000</me:Tmax>
    <me:Tstep>100</me:Tstep>
    <me:withCellDOSCalc/>
  </me:calcMethod>
 </me:control> -->
</me:mesmer>
```

OH + SO_2 Mesmer xml input without vdW complex

```
<?xml version="1.0" encoding="utf-8"?>
<?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>OH+SO2_vdWaals</me:title>
<moleculeList>


<molecule id="OH" description="OH radical">
    <atomArray>
<atom id="a1" elementType="O" x3="0.000000" y3="0.000000" z3="0.107872"/>
<atom id="a2" elementType="H" x3="0.000000" y3="0.000000" z3="-0.862974"/>
</atomArray>
    <bondArray>
     <bond atomRefs2="a1 a2" order="1" />
    </bondArray>
    <propertyList>
     <property dictRef="me:ZPE">
      <scalar units="kJ/mol">0.0</scalar>
     </property>
     <property dictRef="me:rotConsts">
      <array units="cm-1">18.864656</array>
     </property>
     <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
     </property>
     <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.983</scalar>
     </property>
     <property dictRef="me:vibFreqs">
```

```
        <array units="cm-1">3751.964</array>
       </property>
       <property dictRef="me:MW">
        <scalar units="amu">17</scalar>
       </property>
       <property dictRef="me:spinMultiplicity">
        <scalar>2</scalar>
       </property>
       <property dictRef="me:eletronicExcitation">
        <array units="cm-1">139.7</array>
       </property>
     </propertyList>
                <property dictRef="me:eletronicExcitation">
        <array units="cm-1">139.7</array>
       </property>
                <me:DOSCMethod>QMRotors</me:DOSCMethod>
</molecule>


<molecule id="SO2" description="no description">
<atomArray>
<atom id="a1" elementType="S" x3="0.000000" y3="0.000000" z3="0.364946"/>
<atom id="a2" elementType="O" x3="0.000000" y3="1.226750" z3="-0.364946"/>
<atom id="a3" elementType="O" x3="0.000000" y3="-1.226750" z3="-0.364946"/>
</atomArray>
<bondArray>
<bond id="b1" atomRefs2="a1 a2" order="2" />
<bond id="b2" atomRefs2="a1 a3" order="2" />
</bondArray>
<propertyList>
<property title = "SpinMultiplicity" dictRef = "Me:spinMultiplicity">
<scalar>1.0</scalar>
</property>
<property dictRef="me:ZPE">
<scalar units="kJ/mol">0</scalar>
</property>
 <property dictRef="me:frequenciesScaleFactor">
        <scalar>1</scalar>
       </property>
<property dictRef="me:vibFreqs">
<array units="cm-1">544.6479 1254.0399 1444.492 </array>
</property>
<!-- <property title = "Hessian" dictRef = "me:hessian">
<matrix rows="9" matrixType="squareSymmetricLT" units="Hartree/Bohr2">
  4.82802081E-03  4.38154605E-11  1.07143055E+00 -2.30412327E-11  3.69125095E-11
  5.20461675E-01 -2.41401040E-03  5.02028931E-11 -4.38690464E-12  2.40690711E-03
 -4.19097158E-11 -5.35715273E-01  2.71159209E-01 -2.25277576E-11  5.73288760E-01
  9.35206454E-12  3.20017061E-01 -2.60230837E-01  2.17328203E-11 -2.95588135E-01
  2.26060382E-01 -2.41401040E-03  3.30681772E-11  1.62461747E-12  7.10329950E-06
 -1.51709060E-11  2.52248701E-11  2.40690711E-03 -9.77604371E-12 -5.35715273E-01
 -2.71159209E-01 -1.51709419E-11 -3.75734877E-02 -2.44289260E-02 -2.25311660E-11
  5.73288760E-01  1.64532486E-11 -3.20017061E-01 -2.60230837E-01 -2.52247359E-11
  2.44289260E-02  3.41704551E-02 -2.17347477E-11  2.95588135E-01  2.26060382E-01
</matrix>
</property> -->
<property dictRef = "me:rotConsts">
<array units="cm-1">1.97888 0.350165 0.297519 </array>
</property>
 <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
       </property>
                          <property dictRef="me:MW">
        <scalar units="amu">64</scalar>
       </property>
       <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
       </property>
       <property dictRef="me:eletronicExcitation">
        <array units="cm-1">0</array>
       </property>
</propertyList>
```

```
  <me:DOSCMethod>QMRotors</me:DOSCMethod>
</molecule>


<molecule id="TS_1" description="no description">
<atomArray>
<atom id="a1" elementType="S" x3="-0.325857" y3="0.004112" z3="0.295456"/>
<atom id="a2" elementType="O" x3="-0.624891" y3="1.295665" z3="-0.239878"/>
<atom id="a3" elementType="O" x3="-0.983496" y3="-1.137121" z3="-0.248879"/>
<atom id="a4" elementType="O" x3="1.977656" y3="-0.251141" z3="-0.101843"/>
<atom id="a5" elementType="H" x3="2.259567" y3="0.674983" z3="-0.002499"/>
</atomArray>
<bondArray>
<bond id="b1" atomRefs2="a1 a2" order="2" />
<bond id="b2" atomRefs2="a1 a3" order="2" />
<bond id="b4" atomRefs2="a4 a5" order="1" />
</bondArray>
<propertyList>
<property title = "SpinMultiplicity" dictRef = "Me:spinMultiplicity">
<scalar>2.0</scalar>
</property>
<property dictRef="me:ZPE">
<!-- <scalar units="kJ/mol">1.725</scalar> -->

<!-- <scalar units="kJ/mol">1.1</scalar> -->
<scalar units="kJ/mol" lower="-1.00" upper="2.00" stepsize="0.1">-0.2</scalar>
</property>
<property dictRef="me:vibFreqs">
<!-- <array units="cm-1">-225.4756 80.7916 160.6103 220.1169 536.351 601.473 1237.8653 1429.9728 3724.8707 </array> -->
<array units="cm-1">80.7916 160.6103 220.1169 536.351 601.473 1237.8653 1429.9728 3724.8707 </array>
</property>
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 1.05839456E-01 -5.65254837E-01  2.07653298E-01 -1.14967069E-01  6.01777706E-01
-8.94936722E-02  2.43683321E-01 -1.38511048E-01  7.23867974E-02 -2.23896306E-01
 1.18548643E-01 -1.83356729E-01 -2.55443598E-01 -1.46706310E-01  1.42447948E-02
 6.71061059E-03  1.26221664E-02  1.66815034E-01 -2.27360619E-01 -4.67981633E-01
-1.83065592E-01 -2.32015321E-02 -3.62817306E-02 -1.99033009E-02  2.51436040E-01
 5.02698498E-01 -1.60409196E-01 -2.19963793E-01 -1.46530529E-01  1.86411690E-02
 1.57310112E-02  1.91677484E-02  1.36436623E-01  2.02163977E-01  1.26337505E-01
 1.84586454E-02  5.79428772E-03 -9.66185894E-03 -1.76341409E-03  1.51663279E-03
 3.18115197E-03  2.98426081E-03 -2.16963077E-03  2.85113615E-03  3.30965421E-02
 7.49325772E-05 -1.02638687E-02 -3.96145180E-04  2.56999550E-03  1.17181571E-03
-1.10628147E-03 -4.15065432E-03  1.35218302E-03  9.42880542E-04  1.30617835E-01
 4.60115725E-01 -5.22368905E-04 -8.07823152E-04 -5.82827011E-03 -1.79609338E-03
-8.22136906E-04  3.01484881E-03 -2.36358459E-03  4.27971079E-04  1.51554338E-03
 1.59009469E-02  5.13536562E-02  9.68373533E-03 -9.80409813E-04 -8.10343460E-03
-4.99333749E-03  1.21955643E-03  9.00369873E-04  1.30355648E-03 -6.87361277E-04
 1.29574166E-03  2.48026757E-03 -5.27760343E-02 -1.29112109E-01 -1.12189000E-02
 5.32242489E-02 -1.02430922E-03  2.73377662E-03 -2.40454099E-03  3.16400275E-04
-1.41295371E-03  1.22256744E-03  1.44760189E-03  2.12683159E-04  1.12592475E-03
-1.35759125E-01 -4.52375855E-01 -5.01516672E-02  1.35019432E-01  4.50842349E-01
-5.22690943E-04 -1.12468499E-03  3.53914051E-03  3.54548565E-04  1.33413390E-03
-2.22019239E-03  1.11049871E-05  3.76945186E-04 -4.90266842E-04 -1.22713761E-02
-5.07941101E-02 -8.38585745E-03  1.24284134E-02  5.02077160E-02  7.55717620E-03
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</property> -->
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</property>
<property dictRef="me:MW">
       <scalar units="amu">81</scalar>
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<atom id="a2" elementType="O" x3="-1.087253" y3="-0.915565" z3="-0.107052"/>
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-5.64966654E-02 -1.35419603E-01 -2.50807168E-02 -1.32140652E-01  3.24477358E-01
-5.57344892E-02 -4.74165546E-02 -6.61506683E-02  5.45713491E-02  2.37246981E-02
 3.67663556E-02 -3.33679143E-02  9.19929507E-03 -2.33490270E-03 -3.67587331E-01
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-3.45895063E-03  2.39130785E-01 -1.74498899E-01  5.55560298E-03 -2.10739375E-01
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-6.96445161E-03  3.37028346E-03 -1.40832178E-03  1.25767960E-02  3.85176258E-03
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 1.74687219E-02  7.53965849E-03 -2.31998896E-03 -1.59776750E-03  9.29837920E-06
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 1.72337709E-01 -9.36614404E-02 -1.33757796E-01 -5.34915563E-03  6.00947031E-03
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stepsize="0.005" >1.00</me:deltaEDownTExponent> -->
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</me:ExtraDOSCMethod>
</molecule>

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     <molecule ref="SO2" me:type="excessReactant"/>
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    <!-- <me:nInfinity>0.5</me:nInfinity> -->
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            <me:PTs>

             <!--BLITZ2017-->
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<!--WINE-->
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