Temperature and Pressure Dependent Kinetics of QOOH Decomposition and Reaction with O_2: Experimental and Theoretical Investigations of QOOH Radicals Derived from Cl + $(CH_3)_3COOH$

Charlotte A. Whelan, Mark A. Blitz,* Robin Shannon, Lavinia Onel, James P. Lockhart, Paul W. Seakins, Daniel Stone*

School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK

*Corresponding authors

Supporting Information

Analysis of experimental observations

The chemistry occurring within the system can be described through reactions R1-R6, and is summarised in Figure S1.

$(COCl)_2 + h\nu$ ($\lambda = 193$ nm)	→	2 Cl + 2 CO	R1
$(COCl)_2 + h\nu$ ($\lambda = 248$ nm)	→	Cl + CO + COCl	R1a
COCl + M	→	Cl + CO + M	R1b
$(CH_3)_3COOH$ + Cl	→	QOOH + HCl	R2a
$(CH_3)_3COOH$ + Cl	→	$(CH_3)_3CO_2$ + HCl	R2b
QOOH	→	OH + DMO	R3
QOOH + O_2	→	O_2QOOH	R4
$(CH_3)_3COOH + h\nu$ ($\lambda = 193$ nm)	→	$(CH_3)_3CO$ + OH	R5
$(CH_3)_3COOH$ + OH	→	$(CH_3)_3CO_2 + H_2O$	R6

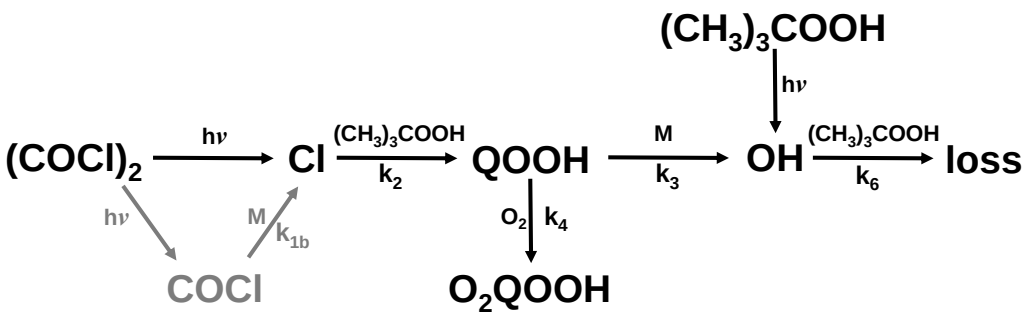

Figure S1: Summary of the relevant chemistry occurring within the reaction system. Processes shown in grey occur only for photolysis at a wavelength of 248 nm.

Production of QOOH radicals is achieved following the photolysis of oxalyl chloride ($(COCl)_2$). At a photolysis wavelength of 193 nm, production of Cl atoms is direct (R1), while at 248 nm the photolysis products include both Cl and COCl (R1a), with subsequent decomposition of COCl producing further Cl atoms (R1b).[1,2] Reaction of Cl atoms with tertiary-butyl hydroperoxide ($(CH_3)_3COOH$) generates QOOH radicals ($CH_2(CH_3)_2COOH$, R2a), which can subsequently undergo decomposition (R3) to produce OH radicals and the cyclic ether dimethyloxirane ($(CH_3)_2C(CH_2)O$, DMO), or, in the presence of O_2, undergo an addition reaction (R4) to produce O_2QOOH radicals ($O_2CH_2(CH_3)_2COOH$). Photolysis of $(CH_3)_3COOH$ also occurs within the system (R5), leading to near-instantaneous production of OH radicals on the timescale of the experiment, with loss of OH radicals from the system occurring as a result of reaction with the $(CH_3)_3COOH$ precursor (R6) and diffusion. The temporal evolution of OH in the system can be used to monitor the reactions of QOOH, as the only non-photolytic source of OH in the system is through decomposition of QOOH, which is in competition with the addition reaction QOOH + O_2.[1]

Determination of the rate coefficients k_3 and k_4 can be achieved through fits to observations of OH temporal profiles. The reactions in the system can be classified as near-instantaneous (for photolysis reactions R1 and R5), first-order (R3), or can be placed under pseudo-first-order conditions (R2, R4 and R6). Thus it is possible to obtain an analytical expression describing the temporal behaviour of OH in the system which can be used to fit the experimental data to find k_3 and k_4. The analytical expression is given by Equation S1:

$$S_{\mathrm{OH}}(t) = S_0 \exp(-k_{1\mathrm{b}}[\mathrm{M}]t) + S_1 \exp(-k'_2 t) + S_2 \exp(-(k_3 + k'_4)\, t) + S_3 \exp(-k'_6 t)$$

(Equation S1)

where $S_{OH}(t)$ is the observed OH fluorescence signal, and is directly proportional to the OH concentration. The rate coefficient k_{1b} is that for the decomposition of COCl, which is constrained in the analysis to previous measurements,[2] k'_2 is the pseudo-first-order rate coefficient for R2 (i.e. $k'_2 = k_2[(CH_3)_3COOH]$), k_3 is the rate coefficient for QOOH decomposition (R3), k'_4 is the pseudo-first-order rate coefficient for R4 ($k'_4 = k_4[O_2]$) since O_2 is in large excess over QOOH, and k'_6 is the pseudo-first-order rate coefficient describing the loss of OH from the system, which, although strictly includes any loss of OH through diffusion, is approximated here as being dominated by R6 (such that $k'_6 = k_6[(CH_3)_3COOH]$).

The coefficient S_0 is linked to the production of Cl, and subsequently OH, through the production and subsequent pressure-dependent decomposition of COCl at a photolysis wavelength of 248 nm. S_0 is given by Equation S2:

$$S_0 = \frac{A_0 k_{1b}[\mathrm{M}] k'_2 k_3}{(k'_2 - k_{1b}[\mathrm{M}])(k_3 + k'_4 - k_{1b}[\mathrm{M}])(k'_6 - k_{1b}[\mathrm{M}])}$$

(Equation S2)

where A_0 corresponds to the photolytic yield of COCl. At 193 nm, A_0 and S_0 are equal to zero and Equation S1 can be simplified to Equation S3:

$$S_{\mathrm{OH}} = S_1 \exp(-k'_2 t) + S_2 \exp(-(k_3 + k'_4)\, t) + S_3 \exp(-k'_6 t)$$

(Equation S3)

The coefficients S_1, S_2 and S_3 in Equations S1 and S2 are linked to the yields of OH through R2, R3 and R5, respectively, through Equations S4-6:

$$S_1 = \frac{k'_2 k_3}{(k_3 + k'_4 - k'_2)(k'_6 - k'_2)}\left(A_1 - \frac{A_0 k_{1b}[\mathrm{M}]}{(k'_2 - k_{1b}[\mathrm{M}])}\right)$$

(Equation S4)

$$S_2 = \frac{k'_2 k_3}{(k_3 + k'_4 - k'_2)}\left(\left(\frac{A_0 k_{1b}[\mathrm{M}]}{(k_3 + k'_4 - k_{1b}[\mathrm{M}])}\right) - A_1\right)\left(\frac{1}{(k'_6 - k_3 - k'_4)}\right)$$

(Equation S5)

$$S_3 = S_4 - S_0 - S_1 - S_2$$

(Equation S6)

where A_1 corresponds to the direct photolytic yield of Cl and S_4 corresponds to the photolytic signal for OH. At 193 nm, Equations S4-S6 simplify to Equations S7-9 since S_0 and A_0 are equal to zero:

$$S_1 = \frac{A_1 k'_2 k_3}{(k_3 + k'_4 - k'_2)(k'_6 - k'_2)}$$

(Equation S7)

$$S_2 = \frac{A_1 k'_2 k_3}{(k_3 + k'_4 - k'_2)(k'_6 - k_3 - k'_4)}$$

(Equation S8)

$$S_3 = S_4 - S_1 + S_2$$

(Equation S9)

Global fits of Equation S1, with the coefficients S_1, S_2 and S_3 described explicitly as detailed above, to experimental observations of OH LIF signals were used in this work to determine the rate coefficients k_3 and k_4. Experiments to determine k_3 were performed in the absence of O_2, with several measurements performed at a single temperature and pressure as a function of the $(CH_3)_3COOH$ concentration to vary the rate of OH loss (i.e. varying k'_6) whilst maintaining the rate of QOOH decomposition between experiments. Typically, experiments were performed with five different concentrations of $(CH_3)_3COOH$, and values for k'_6 were allowed to vary in the fits for each separate dataset whilst fitting k_2 and k_3 as global parameters for each temperature and pressure.

Sensitivity of fits to k_3 and k_4

Given the complexity in the form and derivation of the analytical expression describing the temporal behaviour of OH, a series of simulations of the chemistry occurring in reactions R1-R6 were performed using the numerical integration package Kintecus,[3] with the simulated output for OH analysed in the same manner adopted for experimental data in order to demonstrate the fidelity of the analytical expression in describing the temporal behaviour of OH in the system, and the sensitivity of the fits to k_3 and k_4. The rate coefficients and concentrations used in the simulations are listed in Table S1.

Reaction	Rate coefficient
$(CH_3)_3COOH + Cl \rightarrow QOOH + HCl$	7.7×10^{-11} cm^3 s^{-1}
$QOOH \rightarrow OH + DMO$	35,000 s^{-1}
$QOOH + O_2 \rightarrow O_2QOOH$	7.5×10^{-13} cm^3 s^{-1}
$(CH_3)_3COOH + OH \rightarrow (CH_3)_3CO_2 + H_2O$	3.6×10^{-12} cm^3 s^{-1}

Table S1: Reactions and rate coefficients adopted in simulations of OH used to demonstrate the fidelity and sensitivity of Equation 1 in determinations of k_3 and k_4 (unless otherwise shown as varying in Figures S2-S6). Reactions R1 and R5 are treated as instantaneous, and thus represented by non-zero initial concentrations of Cl, COCl and OH, which were approximated from the absorption cross-sections of $(COCl)_2$ (3.10×10^{-19} cm^2)^2 and $(CH_3)_3COOH$ (1.99×10^{-20} cm^2)^4 at 248 nm, typical laser fluence (10 – 30 mJ cm^{-2}) and typical experimental concentrations of $(COCl)_2$ and $(CH_3)_3COOH$ (1×10^{14} cm^{-3} and 1×10^{15} cm^{-3} respectively). The reaction channel in Cl + $(CH_3)_3COOH$ in which H-abstraction occurs from one of the methyl groups (leading to production of a peroxy radical, RO_2) is not included in the simulations.

Simulations were performed in which the inputs for the rate coefficients k_3 and k'_4 ($k'_4 = k_4[O_2]$) were varied, and the output for OH analysed using Equation S1 to determine the fitted values for k_3 and k'_4. A typical simulation for OH, and the fit to the simulation using Equation S1, is shown in Figure S2. Figures S3 and S4 show the ratios of the fit output for k_3 and k'_4 to the values used as input for the simulation, respectively. Figure S5 shows the ratios of the fit output for k_3 and k'_4 to the input values for a range of $(CH_3)_3COOH$ concentrations. Figure S6 shows the sensitivity of results for k_3 and k_4 to the decomposition rate of COCl (R1b) for experiments performed at a photolysis wavelength of 248 nm. The results demonstrate the fidelity and sensitivity of the analytical expression.

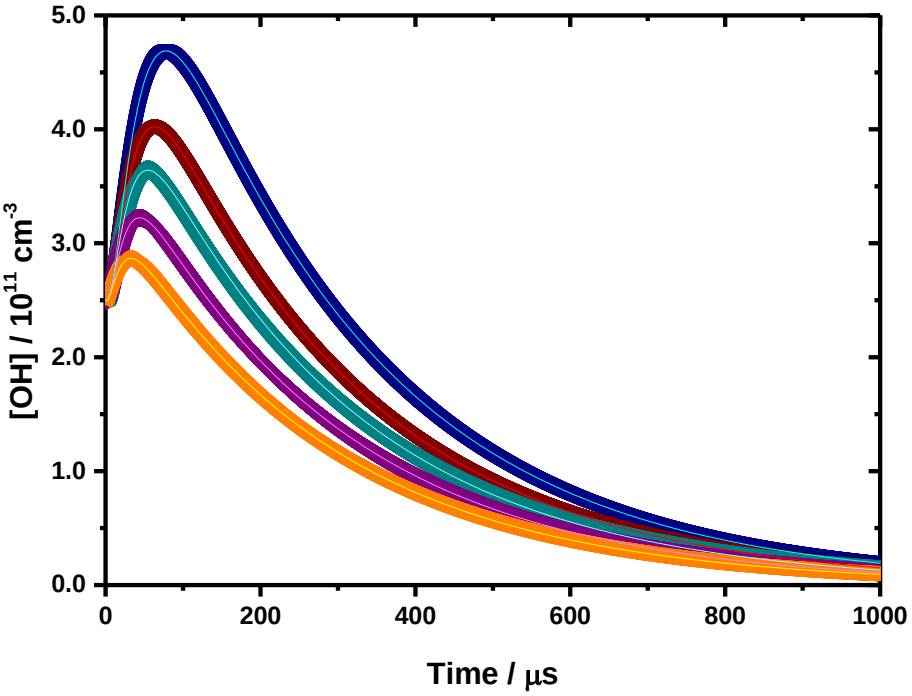

Figure S2: Simulated OH time-profiles (thick lines), using the reactions and rate coefficients listed in Table S1 for a range of O_2 concentrations, and the fit to the simulation using Equation S1 (thin lines).

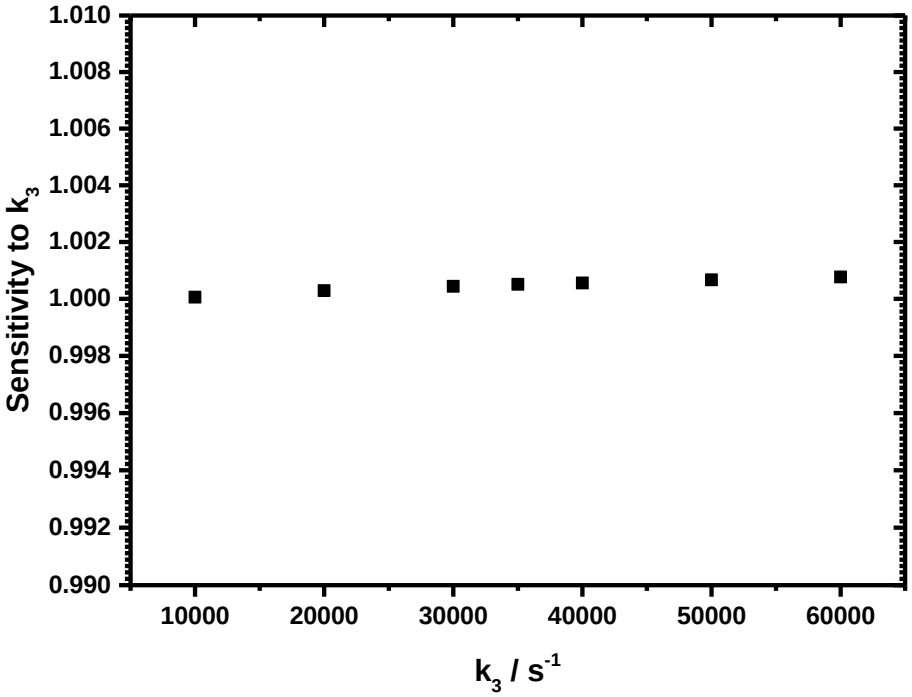

Figure S3: Sensitivity of fits to determine k_3 to the values for k_3 used in the model input (defined as the ratio of the value for k_3 determined by fitting Equation S1 to the output from model simulations of the temporal behaviour of OH to the corresponding value for k_3 used as input in the model).

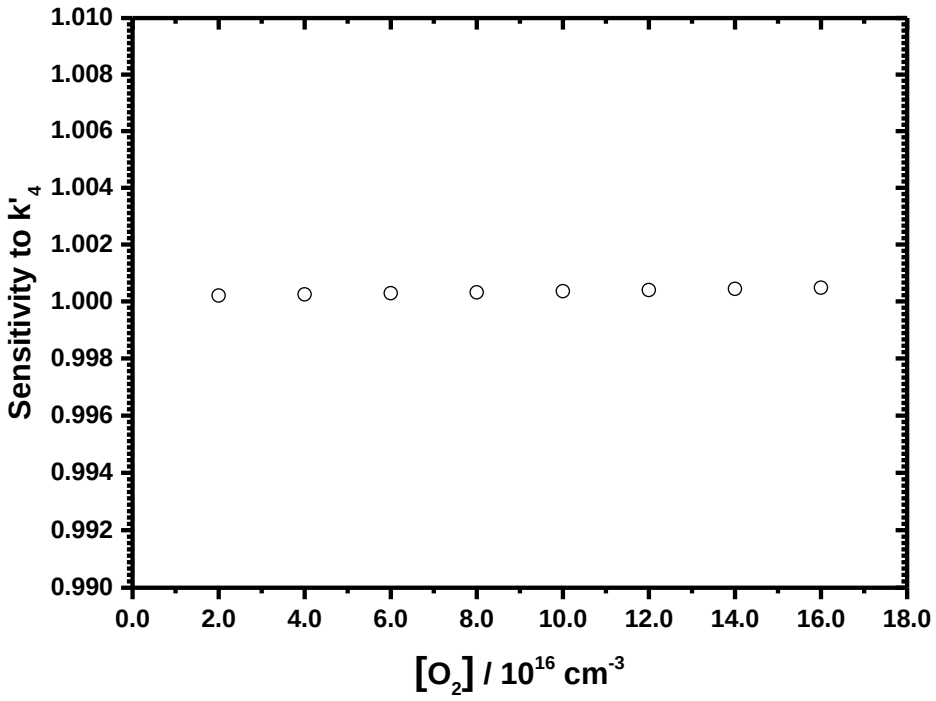

Figure S4: Sensitivity of fits to determine k'_4 to the concentration of O_2 used in the model input (defined as the ratio of the value for k'_4 determined by fitting Equation S1 to the output from model simulations of the temporal behaviour of OH to the corresponding value for k'_4 used as input in the model, where $k'_4 = k_4[O_2]$).

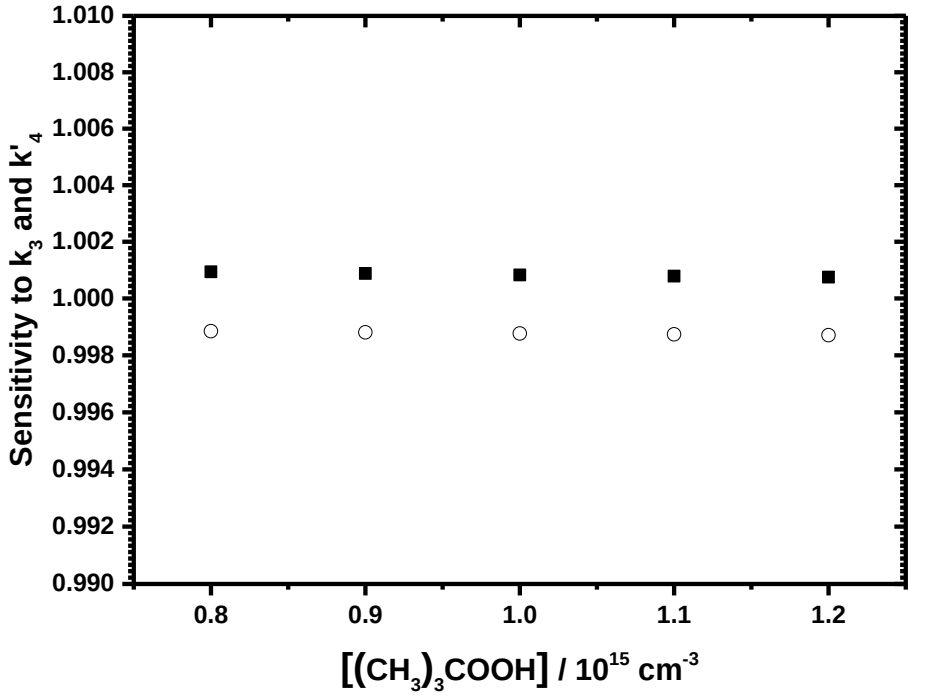

Figure S5: Sensitivity of fits to determine a) k_3 (filled squares) and b) k'_4 (open circles) to those used as inputs for the model simulations of the temporal behaviour of OH occurring as a result of reactions R1-R6 as a function of the initial concentration of $(CH_3)_3COOH$. The sensitivities to k_3 and k'_4 are as defined in Figures S3 and S4, respectively.

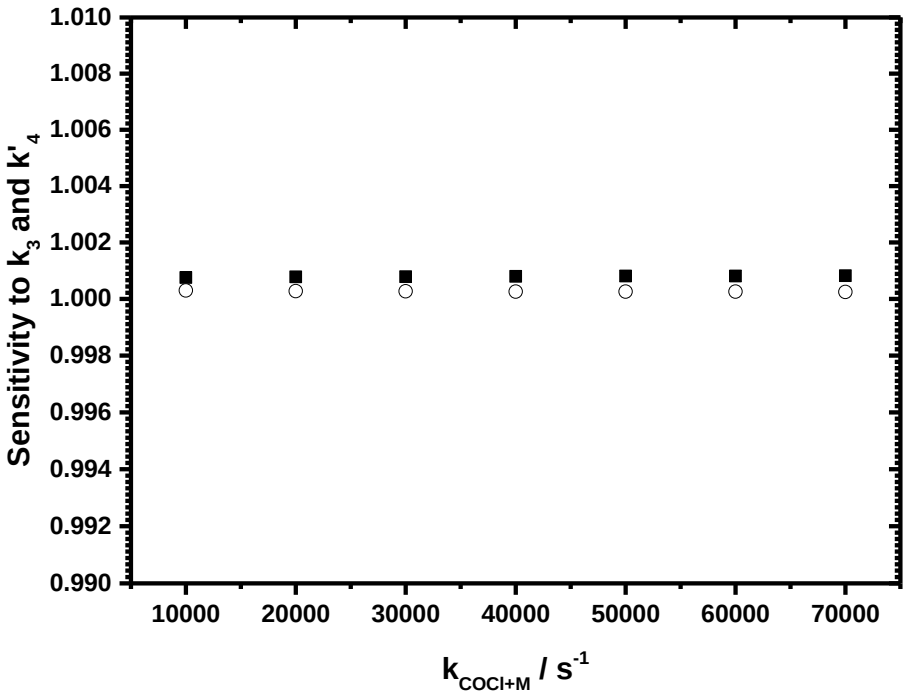

Figure S6: Sensitivity of fits to determine a) k_3 (filled squares) and b) k'_4 (open circles) to those used as inputs for the model simulations of the temporal behaviour of OH occurring as a result of reactions R1-R6 as a function of the rate of COCl decomposition to produce Cl + CO following photolysis of $(COCl)_2$ at a wavelength of 248 nm. The sensitivities to k_3 and k'_4 are as defined in Figures S3 and S4, respectively.

Determination of k_4

Experiments to determine k_4 were performed with varying concentrations of $(CH_3)_3COOH$, (and k'_6 allowed to vary in the fits), with k'_2 varied in the fits as a global parameter and k_3 constrained to the values determined at the relevant temperature and pressure in the absence of O_2. Fits to determine k_4 were performed with data collected at several concentrations of O_2 (typically more than five), either with k'_4 allowed to vary in the fits between datasets, or with the fits constrained to the relevant concentrations of O_2 and k_4 varied as a global parameter in the fit (i.e. k'_4 in the analytical expressions detailed above was replaced by $k_4[O_2]$ with $[O_2]$ constrained). There were no significant differences (< 10 %) between determinations of k_4 in which k'_4 was allowed to vary locally between datasets and those in which k_4 was treated as a global parameter. Figure S7 compares the results obtained for k_4 via the two methods. Results reported for k_4 in the main text are those obtained from the fits to determine k'_4.

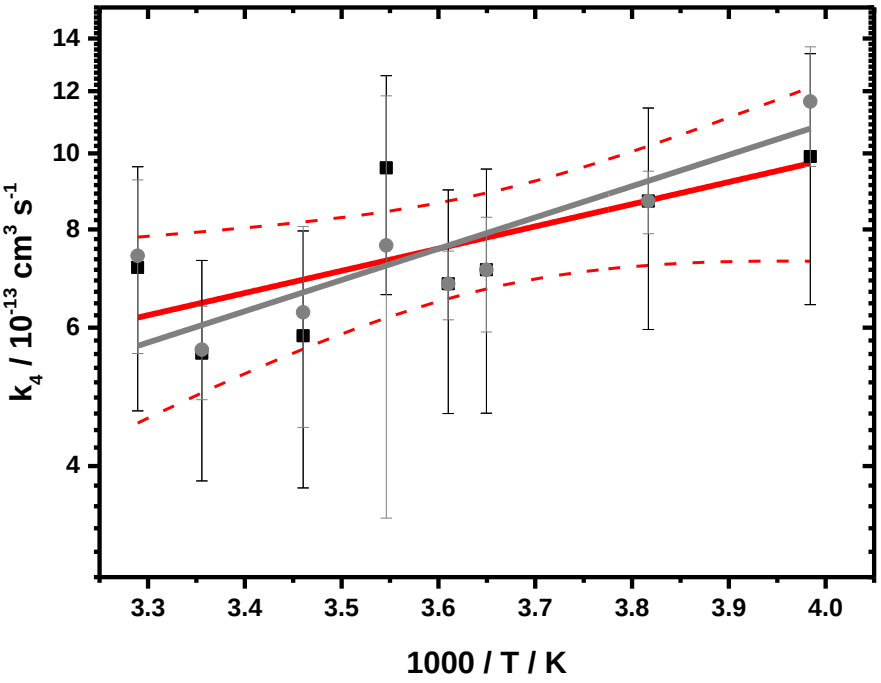

Figure S7: Results for k_4 obtained by fitting data with k'_4 allowed to vary between datasets (black data points), with the Arrhenius fit shown by the solid red line ($A = (7.3 \pm 6.8) \times 10^{-14}$ cm^3 s^{-1} and $E_a = -(5.4 \pm 2.1)$ kJ mol^{-1}), and by fitting data with k_4 treated as a global parameter ((grey data points), with the Arrhenius fit shown by the grey blue line ($A = (2.8 \pm 2.0) \times 10^{-14}$ cm^3 s^{-1} and $E_a = (7.6 \pm 1.6)$ kJ mol^{-1}).

The sensitivity of the fits to the analytical expression used to determine k_4 was investigated by performing fits to the data in which k_4 was fixed to a range of values while k_2 and k_6 were allowed to float. Figure S8 shows the variation in χ^2 for fits performed with different fixed values of k_4 for temperatures between 251 and 298 K. In each case, the minimum in the χ^2 for the fit, which indicates the best fit to the data, corresponds to the value of k_4 determined from the unconstrained fits, giving confidence in the results for k_4.

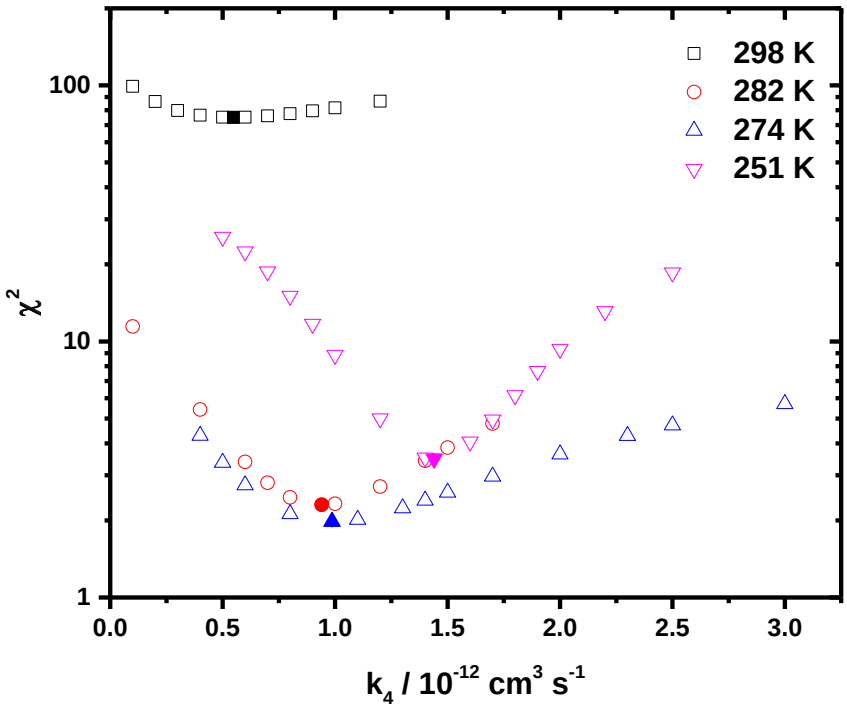

Figure S8: Variation in χ^2 for fits fixed to of k_4 for data at a) 298 K; b) 282 K; c) 274 K; d) 251 K. In each case, the minimum in the χ^2 for the fit, indicating the best fit to the data, corresponds to the value of k_4 determined by the unconstrained fit (shown by filled symbols).

Results for k_2 and k_6

Figures S9 and S10 show the results for k_2 and k'_6, respectively, which are also summarised in Table S2. Results for k_2 can be parameterised by the Arrhenius parameters $A = (2.3 \pm 2.1) \times 10^{-12}$ cm^3 s^{-1} and $-E/R = (690 \pm 250)$ K, while k_6 can be parameterised by the Arrhenius parameters $A = (1.0 \pm 0.7) \times 10^{-13}$ cm^3 s^{-1} and $-E/R = (890 \pm 210)$ K.

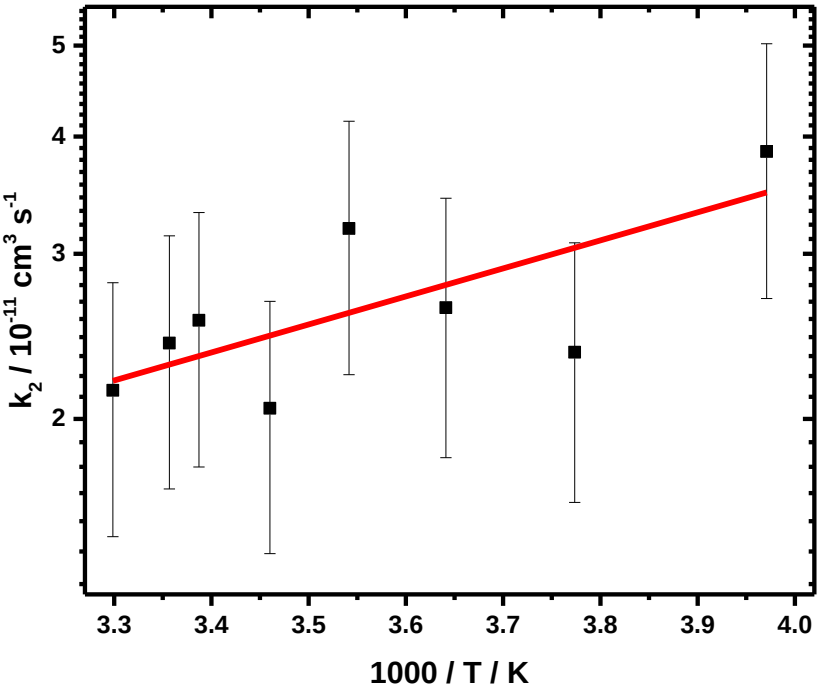

Figure S9: Temperature dependence of k_2, the rate coefficient for reaction of Cl with $(CH_3)_3COOH$ observed in this work (black points) with Arrhenius parameterisation (solid red line).

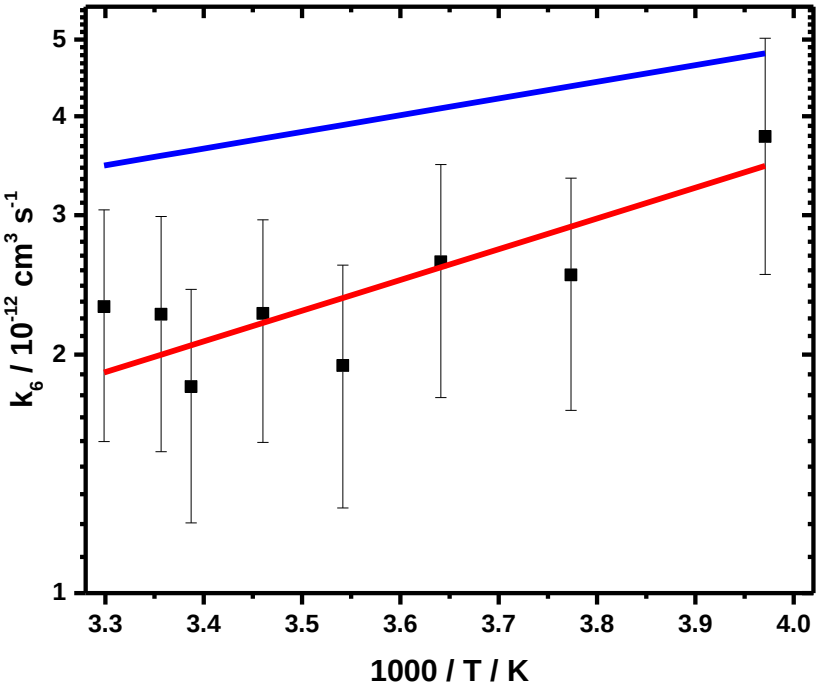

Figure S10: Temperature dependence of k_6, the rate coefficient for reaction of OH with $(CH_3)_3COOH$ observed in this work (black points) with Arrhenius parameterisation (solid red line). The parameterisation for k_6 reported by Baasandorj et al.[4] is also shown (solid blue line).

T / K	k_2 / 10^{-11} cm^3 s^{-1}	k_6 / 10^{-12} cm^3 s^{-1}
304	2.2 ± 0.6	2.3 ± 0.7
298	2.4 ± 0.7	2.3 ± 0.7
289	2.1 ± 0.6	2.3 ± 0.7
282	3.2 ± 1.0	1.9 ± 0.7
275	2.6 ± 0.8	2.6 ± 0.9
265	2.4 ± 0.7	2.5 ± 0.8
251	3.9 ± 1.2	3.8 ± 1.3

Table S2: Summary of results for k_2 (Cl + $(CH_3)_3COOH$) and k_6 (OH + $(CH_3)_3COOH$) as a function of temperature.

While the results of Baasandorj et al.[4] indicate that the reaction of OH with $(CH_3)_3COOH$ (R6) proceeds exclusively via abstraction from the OO-H bond, experiments were also performed in this work to investigate the possibility of QOOH production and regeneration of OH from R6. If QOOH were produced via the reaction of OH with $(CH_3)_3COOH$, with subsequent production of OH via decomposition of QOOH (R3), the observed decay kinetics of OH in the system and thus values for k'_6 determined in our analysis, would vary with the concentration of O_2. Figure S11 shows the values for k'_6 determined in this work in experiments in which the concentrations of O_2 were varied, indicating that the loss of OH in the system is independent of O_2 and that $(CH_3)_3CO_2$ is the sole product of R6, with no production of QOOH occurring via abstraction from one of the C-H bonds.

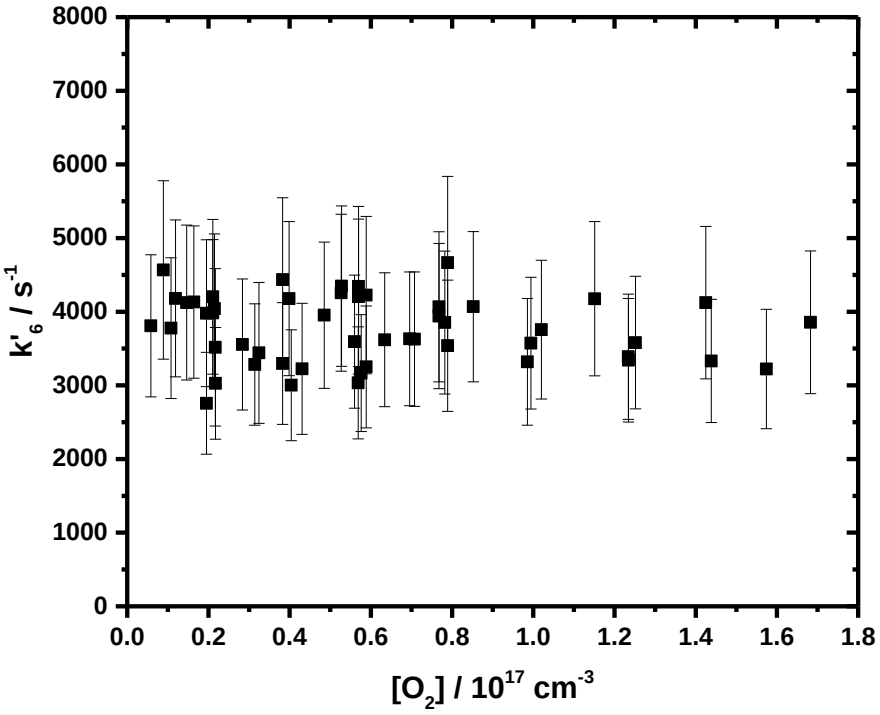

Figure S11: Variation of the rate coefficient describing the loss of OH in the system (k'_6) as a function of the O_2 concentration for experiments performed at 298 K with similar $(CH_3)_3COOH$ concentrations.

MESMER analysis of k_3

The barrier height for QOOH decomposition of 44.7 kJ mol^{-1} was determined by fitting the experiment results for k_3 obtained in this work using the Master Equation Solver for Multi-Energy well Reactions (MESMER).[5] The value obtained is slightly lower than that reported by Zádor et al.[1] from high level calculations (52.3 kJ mol^{-1}) and that determined by comparison with experimental data obtained in He between 8 and 90 Torr at 298 K (48.1 kJ mol^{-1}). The results reported by Zádor et al. underestimate the observations for k_3 made in this work, as shown in Figure S12.

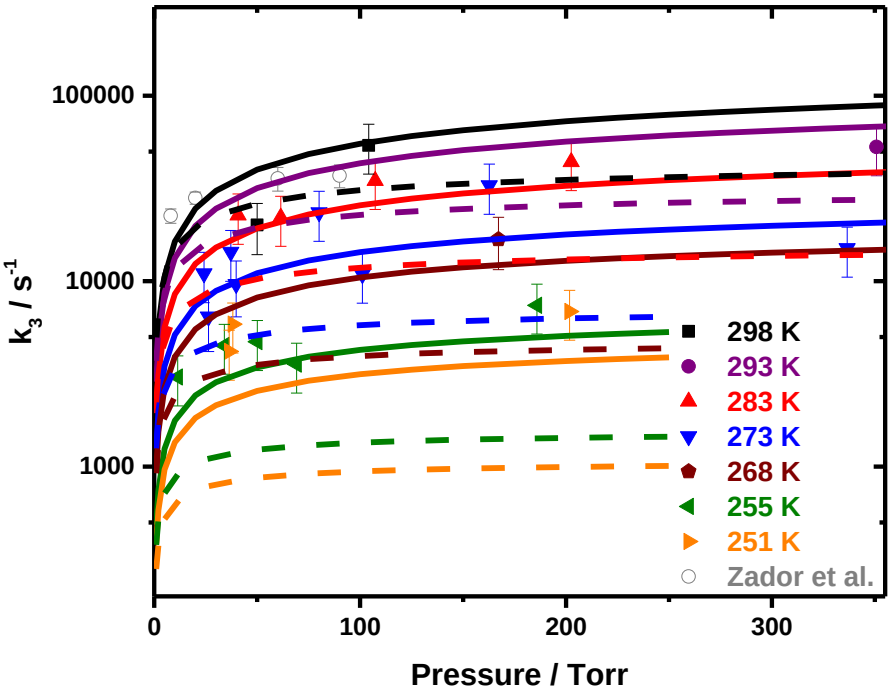

Figure S12: Pressure dependence of k_3 from in He bath gas observed in this work (filled data points) and by Zádor et al. (open data points). Solid lines are the MESMER fits to the observations made in this work, which gave a barrier height to decomposition of 44.7 kJ mol^{-1} and ΔE_{down} = 89 cm^{-1} in He. Broken lines are MESMER simulations using a barrier height of 48.1 kJ mol^{-1} and ΔE_{down} = 250 cm^{-1}, as reported by Zádor et al.[1]

Figure S13 shows fits to the results of Zádor et al. performed using MESMER, which indicated that a barrier height of 48.1 kJ mol^{-1} required a value for $\langle\Delta E\rangle_{down}$ greater than 600 cm^{-1}, with fits constrained to the barrier of 44.7 kJ mol^{-1} determined in this work giving an optimum $\langle\Delta E\rangle_{down}$ of 94 cm^{-1}. Fits constrained to the value for $\langle\Delta E\rangle_{down}$ used in the work of Zádor et al. (250 cm^{-1}) gave an optimum barrier height of 47.1 kJ mol^{-1}, while fits constrained to $\langle\Delta E\rangle_{down}$ = 89 cm^{-1}, as determined in this work for He, gave an optimum barrier height of 44.8 kJ mol^{-1}.

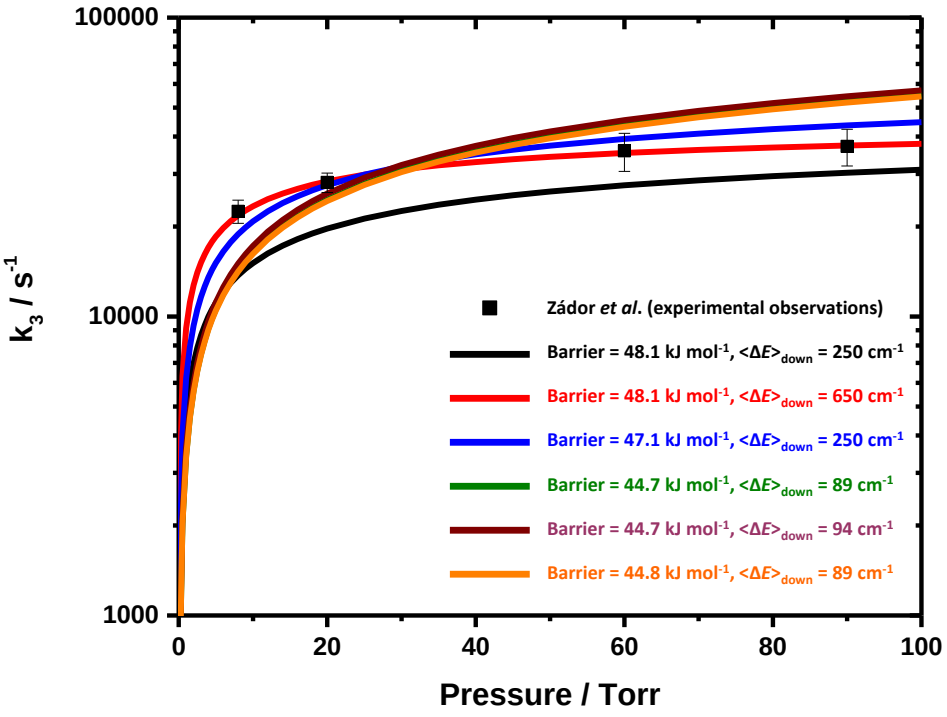

Figure S13: Results for k_3 at 298 K reported by Zádor et al.[1] and corresponding output from MESMER for simulations (black line, barrier to decomposition of 48.1 kJ mol^{-1} and $\langle\Delta E\rangle_{down}$ = 250 cm^{-1}) and fits to the results of Zádor et al. (coloured lines).

MESMER simulations were performed using the barrier height determined in this work (44.7 kJ mol-1) and values for $\langle\Delta E\rangle_{down}$ in He (89 cm^{-1}) and N_2 (147 cm^{-1}) to calculate k_3 at temperatures between 200 and 800 K and pressures between 1 and 10^6 Torr. The output was parameterised using the Troe expression for broad falloff curves,[6] as detailed in the main text. Figure S14 shows the fits to the MESMER output to provide the parameterisation.

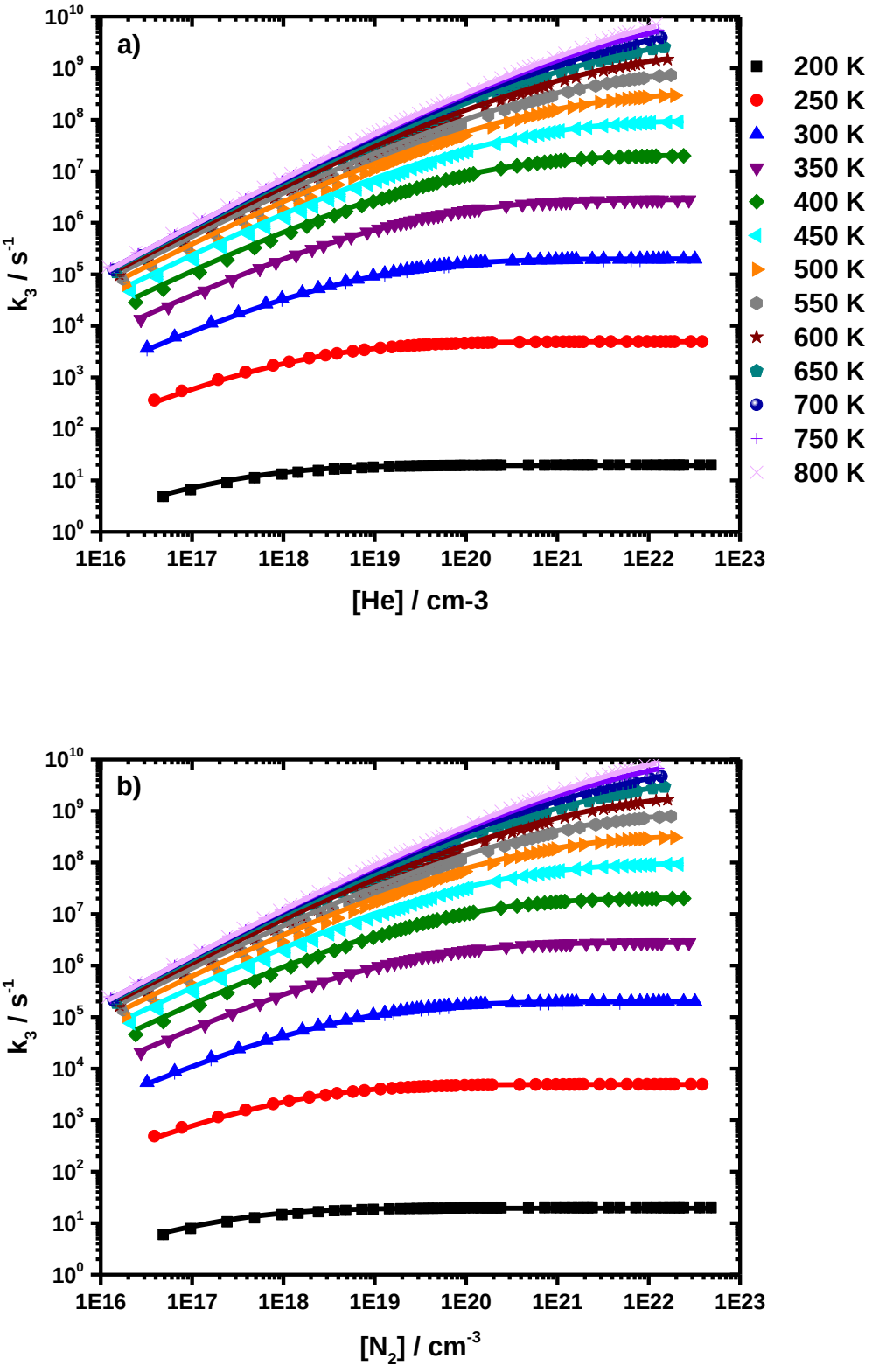

Figure S14: Troe fits using Equations 3-6 in the main text (solid lines) to MESMER simulations (filled data points) using a barrier height of 44.7 kJ mol^{-1} in a) He, with $\langle\Delta E\rangle_{down}$ =89 cm^{-1} and b) N_2, with $\langle\Delta E\rangle_{down}$ = 147 cm^{-1}.

References

(1) Zador, J.; Huang, H. F.; Welz, O.; Zetterberg, J.; Osborn, D. L.; Taatjes, C. A., Directly measuring reaction kinetics of QOOH – a crucial but elusive intermediate in hydrocarbon autoignition, Phys. Chem. Chem. Phys. 2013, 15, 10753-10760.

(2) Ghosh, B.; Papanastasiou, D. K.; Burkholder, J. B., Oxalyl chloride, ClC(O)C(O)Cl: UV/vis spectrum and Cl atom photolysis quantum yields at 193, 248, and 351 nm, J. Chem. Phys. 2012, 137, 164315, 1-12.

(3) Ianni, J. C., Kintecus, Windows Version 2.80, www.kintecus.com 2002.

(4) Baasandorj, M.; Papanastasiou, D. K.; Talukdar, R. K.; Hasson, A. S.; Burkholder, J. B., $(CH_3)_3COOH$ (tert-butyl hydroperoxide): OH reaction rate coefficients between 206 and 375 K and the OH photolysis quantum yield at 248 nm, Phys. Chem. Chem. Phys. 2010, 12, 12101-12111.

(5) Glowacki, D. R.; Liang, C.-H.; Morley, C.; Pilling, M. J.; Robertson, S. H., MESMER: An open-source master equation solver for multi-energy well reactions, J. Phys. Chem. A 2012, 116, 9545-9560.

(6) Troe, J.; Ushakov, V.G., Representation of "broad" falloff curves for dissociation and recombination reactions, Z. Phys. Chem. 2014, 228, 1, 1-10.

MESMER Input File

```
<?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>QOOH decomposition</me:title>
  <moleculeList>

    <molecule xmlns="http://www.xml-cml.org/schema" id="QOOH">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.000171" y3="-0.001516" z3="0.005092"/>
        <atom id="a2" elementType="H" x3="0.024675" y3="0.009510" z3="1.093773"/>
        <atom id="a3" elementType="H" x3="1.022636" y3="-0.005037" z3="-0.372849"/>
        <atom id="a4" elementType="H" x3="-0.501226" y3="-0.908348" z3="-0.325736"/>
        <atom id="a5" elementType="C" x3="-0.734094" y3="1.229700" z3="-0.507006"/>
        <atom id="a6" elementType="C" x3="-0.093414" y3="2.516850" z3="0.009170"/>
        <atom id="a7" elementType="H" x3="0.933881" y3="2.581690" z3="-0.345923"/>
        <atom id="a8" elementType="H" x3="-0.645690" y3="3.385071" z3="-0.347691"/>
        <atom id="a9" elementType="H" x3="-0.095366" y3="2.520449" z3="1.098720"/>
        <atom id="a10" elementType="C" spinMultiplicity="2" x3="-0.834202" y3="1.244012" z3="-1.997167"/>
        <atom id="a11" elementType="H" x3="-1.290598" y3="2.091894" z3="-2.488619"/>
        <atom id="a12" elementType="H" x3="-0.465578" y3="0.425829" z3="-2.596208"/>
        <atom id="a13" elementType="O" x3="-2.054784" y3="1.298273" z3="0.074548"/>
        <atom id="a14" elementType="O" x3="-2.785316" y3="0.139167" z3="-0.287679"/>
        <atom id="a15" elementType="H" x3="-3.253439" y3="0.434038" z3="-1.077776"/>
      </atomArray>
      <bondArray>
        <bond atomRefs2="a12 a10" order="1"/>
        <bond atomRefs2="a11 a10" order="1"/>
        <bond id ="b4" atomRefs2="a10 a5" order="1"/>
        <bond atomRefs2="a15 a14" order="1"/>
        <bond id ="b3" atomRefs2="a5 a1" order="1"/>
        <bond id="b5" atomRefs2="a5 a6" order="1"/>
        <bond id="b2" atomRefs2="a5 a13" order="1"/>
        <bond atomRefs2="a3 a1" order="1"/>
        <bond atomRefs2="a8 a6" order="1"/>
        <bond atomRefs2="a7 a6" order="1"/>
        <bond atomRefs2="a4 a1" order="1"/>
        <bond id="b1" atomRefs2="a14 a13" order="1"/>
```

<bond atomRefs2="a1 a2" order="1"/>
<bond atomRefs2="a6 a9" order="1"/>
</bondArray>
<propertyList>
<property title="program">
<scalar>Gaussian 09, Revision D.01</scalar>
</property>
<property title="basis">
<scalar>6-311+G(3d,2p) (5D, 7F)</scalar>
</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kJ/mol" >0 </scalar>
</property>
<property title="Hessian" dictRef="me:hessian">
<matrix rows="45" matrixType="squareSymmetricLT" units="Hartree/Bohr2">0.56240319 0.04403545 0.52374075 -0.01875606 0.03038503 0.58393575 -0.04722566 -0.00092655 -0.00382439 0.04646554 -0.00009031 -0.04816916 -0.00780923 -0.00163048 0.05110010 -0.00584605 -0.00457823 -0.31870812 0.00663838 0.00411350 0.34582306 -0.28322471 0.00071975 0.08711921 0.00256152 -0.00018240 -0.00073926 0.30797992 -0.00165399 -0.04687814 0.00156926 0.00052307 -0.00153511 -0.00030892 -0.00087546 0.04933068 0.08864969 0.00042997 -0.08029360 0.03081644 0.00002895 -0.00882130 -0.09659538 -0.00146119 0.08277805 -0.10559415 -0.10832432 -0.03990765 -0.00049447 0.00133828 0.00037771 -0.01273172 -0.02494522 -0.01036622 0.11329160 -0.10500204 -0.23563222 -0.06959022 0.00093865 0.00078440 0.00029535 0.00098286 0.00165630 0.00121692 0.11553915 0.25727571 -0.03968554 -0.07062022 -0.07525083 -0.01559779 -0.02724058 -0.00822757 0.00484527 0.01107178 0.00296685 0.04439839 0.07520643 0.07716692 -0.09445053 0.04359997 -0.02336563 -0.00168891 -0.00049405 0.00080508 -0.01384090 0.02313139 -0.00986468 0.00863035 -0.01350387 0.00731828 0.41475348 0.03807263 -0.16094714 0.03843959 0.00022631 -0.00053949 -0.00084263 -0.00350989 0.00179098 -0.00111892 0.01435482 -0.02291063 0.00984245 -0.02822739 0.53557790 -0.02166443 0.03542731 -0.09714415 -0.01732005 0.02871961 -0.01306788 0.00676046 -0.01109284 0.00229448 0.00569107 -0.00892326 0.00257453 0.03674542 0.00611151 0.52119623 0.00976779 0.01301759 0.00502271 -0.00003465 -0.00009468 0.00024895 0.00014441 -0.00001440 0.00011086 -0.00188442 0.00392823 -0.00123893 -0.08726187 -0.02935402 -0.01274455 0.57395340 -0.01017347 -0.03219491 -0.00814499 -0.00092178 0.00146768 -0.00095719 -0.00098838 0.00110886 -0.00040839 0.00224403 -0.00339463 0.00142615 -0.03619445 -0.15593588 -0.02696257 -0.03999806 0.50611147 0.00556314 0.00909105 0.00421891 0.00013753 0.00113626 0.00036097 0.00024656 -0.00062736 0.00004557 -0.00101438 0.00273187 -0.00058526 -0.02529145 -0.03954501 -0.09086191 -0.01776778 -0.03618050 0.57128323 0.00011509 0.00090216 0.00028450 0.00000150 -0.00007213 -0.00012319 0.00067055 -0.00012622 -0.00001909 0.00023392 0.00000475 -0.00025967 -0.01252950 0.00204494 0.00493277 -0.28910290 -0.01472357 0.08459104 0.31350253 -0.00015162 0.00113350 0.00043039 0.00001092 -0.00006326 0.00005972 0.00029562 -0.00079164 -0.00016478 0.00015038 0.00030390 -0.00014421 -0.02515915 0.00009034 0.01105884 -0.01234662 -0.04698404 0.00434346 0.01654777 0.05035249 0.00009775 0.00033911 -0.00001901 0.00018843 -0.00000302 -0.00004146 0.00001476 0.00010454 0.00027144 -0.00015331 0.00010030 -0.00010834 -0.01137927 0.00043140 0.00252493 0.08589251 0.00513083 -0.07537204 -0.09255335 -0.00388548 0.07861907 -0.00113294 -0.00183407 -0.00057396 -0.00014442 -0.00001209 -0.00006155 0.00026197 -0.00022137 -0.00013365 0.00053787 -0.00069343 0.00003121 0.00652751 -0.01162685 0.00539039 -0.11832502 0.11152033 -0.04682074 -0.01387812 0.02418059 -0.01115964 0.12496133 -0.00406505 -0.00383028 -0.00278085 -0.00008244 0.00023898 -0.00003339 0.00001352 0.00029487 -0.00008753 0.00099313 -0.00142338 0.00059765 0.01546371 -0.02336165 0.00998204 0.10923100 -0.21610522 0.07083272 -0.00173355 0.00281998 -0.00177656 -0.11970485 0.23710759 -0.00111113 -0.00174889 -0.00058378 0.00001815 -0.00029514 0.00037910 -0.00025756 0.00012174 -0.00007430 0.00011496 -0.00057835 0.00078144 0.00718852 -0.00891369 0.00230393 -0.04721620 0.07219289 -0.07877001 0.00507348 -0.00981814 0.00289914 0.05202417 -0.07671434 0.08117682 -0.00011552 0.00078133 0.00029347 0.00036687 0.00009597 0.00019041 0.00000065 0.00003657 0.00015952 -0.00012620 0.00006598 -0.00002306 -0.00190112 -0.00026639 -0.01509001 -0.04697471 0.00111117 0.00216354 0.00186967 0.00008290 0.03096558 -0.00024242 -0.00112981 -0.01704506 0.04655594 0.00019393 0.00161659 -0.00101068 0.00000745 -0.00068063 0.00047650 0.00003549 -0.00011431 0.00005459 -0.00007860 0.00024825 0.00035048 -0.00070210 -0.00165182 -0.02997454 0.00085315 -0.04770201 0.00332165 0.00036892 -0.00131031 0.00191737 -0.00165834 0.00080705 0.02580104 0.00109292 0.05081633 0.00019183 0.00090178 0.00041288 0.00025508 -0.00041178 0.00060940 -0.00012270 -0.00004417 0.00001565 -0.00009469 0.00003419 0.00036327 -0.00028252 0.00033587 -0.01246637 0.00062462

0.00147265 -0.31721346 -0.00058038 0.00020414 -0.00829611 0.00049718 -0.00034781 -0.00865664 -0.00065948 -0.00025015 0.34474641 -0.00037811 0.00123921 -0.01840155 -
0.00114391 0.00297254 -0.00126656 0.00053631 -0.00050450 -0.00011481 0.00023769 -0.00007635 0.00023885 -0.05249162 0.01726169 -0.01993265 0.00016521 -0.00119527 -
0.01147970 0.00067211 0.00041568 -0.00034916 0.00023345 0.00008523 0.00103436 0.00021413 -0.00155296 -0.00063663 0.18321249 0.00393683 -0.00205373 0.03108829 0.00302097 -
0.00451294 0.00243242 0.00020451 0.00044476 0.00007248 -0.00029851 0.00080786 0.00058817 0.02061473 -0.08180899 0.00277960 -0.00305908 -0.00242341 -0.02788222 0.00029148
0.00054214 0.00009697 -0.00001204 0.00082159 -0.00086490 -0.00217340 -0.00377148 -0.00271245 -0.23486787 0.53607788 -0.00647121 0.00465696 -0.01816196 -0.00070624
0.00110130 0.00020009 0.00057993 -0.00018399 -0.00002152 0.00060743 -0.00147459 0.00097311 -0.02478716 0.00701055 -0.21844278 -0.00531010 -0.00995859 -0.01930889
0.00038883 0.00064489 -0.00006515 0.00068854 0.00158275 0.00084131 -0.00057217 -0.00075348 -0.00043686 0.01453737 0.02532189 0.54521740 0.00078023 -0.00050011 -0.00060029
0.00008188 0.00023837 -0.00018092 0.00007945 -0.00002562 -0.00002008 0.00000289 0.00000169 0.00016247 -0.00054059 0.00155594 0.00041071 0.00029019 0.00072608 0.00032992 -
0.00024781 -0.00002011 -0.00014020 0.00011202 -0.00018892 -0.00022413 -0.00011352 -0.00012370 0.00020657 -0.07030084 0.11478730 -0.05716873 0.06921194 -0.00022275
0.00080796 0.00028983 0.00005935 0.00021365 0.00004044 -0.00015585 0.00004454 -0.00021337 0.00006356 0.00024528 -0.00014874 -0.00031627 0.00115935 -0.00292254 -0.00010819
0.00114839 -0.00018682 -0.00009733 -0.00007734 0.00008052 0.00014813 0.00024804 -0.00000141 -0.00005236 0.00005850 0.00012487 0.11586412 -0.22811374 0.10149379 -
0.12129476 0.23401311 0.00060184 -0.00162971 -0.00565515 -0.00095115 0.00158713 -0.00051914 -0.00021249 -0.00012185 0.00011184 0.00015132 0.00007939 0.00003488 -
0.01412839 0.02373907 -0.00640094 0.00027185 0.00149724 0.00127930 -0.00005651 -0.00010722 -0.00003214 0.00005712 -0.00090737 -0.00023304 0.00020475 -0.00025254
0.00014904 -0.05714651 0.09967587 -0.11499325 0.06319835 -0.11010871 0.11395203 -0.00009087 -0.00014152 -0.00044450 -0.00001109 -0.00007537 0.00010346 -0.00008206 -
0.00005659 -0.00017507 0.00017491 -0.00016548 0.00022151 0.00461089 -0.00085441 -0.00244538 -0.00061374 -0.00092840 -0.00053571 -0.00007461 -0.00006531 0.00000091
0.00000051 -0.00002949 -0.00010889 -0.00011125 -0.00008230 -0.00030049 -0.05146604 0.09784542 0.05377921 -0.00035807 0.00693765 0.00703548 0.04937694 0.00009672
0.00090404 0.00061576 -0.00005205 0.00003285 0.00000091 -0.00018423 0.00013732 -0.00012358 -0.00028110 0.00004094 -0.00017575 0.00021283 0.00367222 0.00342503 0.00003662
-0.00024652 0.00001719 -0.00009979 -0.00007344 -0.00006128 -0.00002987 0.00033252 0.00010162 -0.00012656 0.00027422 -0.00014760 0.09905266 -0.21896043 -0.12606275
0.00527835 -0.00956563 -0.01274543 -0.10206762 0.22354943 0.00073643 -0.00124516 0.00127937 -0.00001379 0.00013570 0.00039572 -0.00051989 0.00008886 -0.00023222
0.00018115 0.00071382 -0.00028572 0.00812834 -0.02047513 -0.00498901 0.00033892 0.00115166 -0.00319940 -0.00020406 -0.00015237 0.00002490 0.00007136 -0.00005287
0.00004413 -0.00053334 -0.00092655 -0.00041442 0.05323981 -0.12401331 -0.14565750 -0.00515894 0.01106050 0.01013048 -0.05772161 0.13389077 0.14688197 -0.04069187
0.00566611 0.01310040 0.00159947 -0.00189682 0.00027902 -0.00280130 0.00628067 -0.00221423 0.00103816 -0.00129294 0.00045470 -0.14745139 0.04574155 0.05157501 -0.02924440
-0.01300944 0.00308935 -0.00046667 -0.00068963 -0.00034539 0.00071508 0.00135847 0.00030417 0.00017490 0.00085279 0.00068709 -0.00988524 0.00004287 0.02344790 0.00130949
-0.00032171 0.00039449 -0.00095958 -0.00142808 0.00094157 0.34825148 0.03178033 0.00121062 -0.01394226 -0.00101050 0.00183843 -0.00073394 0.00300483 -0.00631182
0.00140733 -0.00156117 0.00004588 -0.00105589 0.01174241 -0.08194988 -0.01500371 -0.03714612 -0.00875663 0.00841491 -0.00278113 -0.00464223 -0.00139683 -0.00057287
0.00136302 0.00078594 -0.00019653 0.00101043 0.00081186 0.00128093 0.00249001 -0.00283465 -0.00015757 0.00024340 -0.00137921 -0.00047579 0.00029018 -0.00086855 0.08344792
0.30004593 -0.00187931 -0.00081248 0.00563810 0.00008957 -0.00129210 0.00175597 -0.00147014 0.00093687 0.00089448 0.00035421 -0.00025835 -0.00028722 0.04745537 -
0.02601369 -0.08999235 -0.00968493 -0.00122127 0.00768767 -0.00179883 -0.00231291 -0.00135827 -0.00017328 -0.00004486 0.00002902 -0.00055209 0.00076862 0.00060304
0.03695756 -0.01082331 -0.02985352 -0.00086327 0.00032375 0.00223635 0.00060597 0.00113768 -0.00494383 -0.03617854 0.11018523 0.17773391 0.00011857 0.00179554 -0.00024506
-0.00046794 -0.00006000 -0.00058948 0.00045106 -0.00151485 -0.00020232 -0.00311451 -0.00073227 -0.00061193 -0.01959827 -0.04513018 -0.01681521 -0.01034795 0.00283812
0.00610910 -0.00073927 -0.00302319 -0.00115223 0.00034502 -0.00014556 0.00026865 0.00028322 0.00054108 -0.00000182 -0.00033379 -0.00068409 0.00039737 -0.00011956 -
0.00017073 0.00034344 0.00009920 -0.00035269 0.00026337 -0.10669191 -0.08534250 -0.01690922 0.26357321 0.00313839 0.00071123 0.00050809 -0.00006343 -0.00000654 0.00007978
0.00060298 0.00057951 0.00036760 0.00066374 0.00175332 -0.00001472 -0.01168631 -0.01193612 0.00085101 -0.00387874 0.00375690 0.00403074 -0.00042455 -0.00093224 -
0.00120969 0.00048746 0.00080695 -0.00007465 0.00056027 0.00025798 -0.00016292 0.00019839 -0.00007891 -0.00108860 -0.00005038 -0.00000872 0.00029684 -0.00017539 -
0.00017408 0.00045353 -0.08952455 -0.20094507 -0.03006708 0.04479423 0.30463100 -0.00105309 -0.00042199 0.00100136 0.00035116 0.00012739 -0.00007905 0.00012011 0.00006978
-0.00002016 -0.00036034 0.00042723 -0.00021770 0.00298620 0.01046992 -0.00152590 0.00057754 0.00091378 0.00128778 0.00005790 -0.00038703 0.00082233 0.00023064 -0.00019800
-0.00019522 0.00060866 0.00064292 0.00068367 0.00434541 0.00407816 0.00017338 -0.00030914 -0.00026400 0.00029638 -0.00031048 -0.00001888 0.00124374 -0.05315625 -
0.08098234 -0.06388228 0.23771447 -0.10410395 0.40829348 -0.00028050 -0.00003054 0.00029880 0.00013428 -0.00003684 0.00016402 -0.00000514 -0.00003347 -0.00003099 -
0.00020191 0.00000507 -0.00025377 -0.00276752 -0.00028878 -0.00549354 -0.00053135 -0.00030690 0.00067958 -0.00002647 -0.00022822 0.00007262 0.00002816 -0.00006537 -
0.00006350 0.00011936 0.00025226 0.00021634 0.00072818 0.00035088 0.00058905 -0.00018768 -0.00033285 0.00023640 -0.00049513 -0.00005518 0.00025069 -0.01489622 -0.00201223
-0.01595307 -0.12345708 0.05535789 -0.19180278 0.14183903 0.00010495 -0.00041912 -0.00004800 -0.00009951 -0.00016895 -0.00004434 0.00003666 0.00024321 -0.00000008
0.00014183 0.00019901 0.00031702 0.00151856 -0.00124920 -0.00347550 -0.00106667 0.00014993 0.00050206 -0.00010175 -0.00036786 0.00013181 0.00002928 -0.00012007 0.00000630
0.00011794 0.00014121 0.00019153 -0.00017351 0.00053937 0.00054452 -0.00022655 -0.00041681 0.00037650 0.00033460 -0.00021363 0.00023910 -0.03522721 -0.00593228 -

0.04050610 0.08718709 -0.09841521 0.16964702 -0.05257571 0.10603039 0.00062615 -0.00017452 -0.00066977 -0.00008133 0.00010201 -0.00005977 0.00023112 -0.00012251
0.00008474 0.00002036 0.00001929 0.00010163 -0.00152810 0.00052872 0.00399720 0.00087454 0.00004830 -0.00085247 0.00026658 0.00023071 0.00013073 -0.00006777 -0.00005157
0.00005810 -0.00011072 -0.00016523 -0.00009948 -0.00102579 0.00016233 -0.00046384 0.00035768 0.00043188 -0.00035663 0.00029558 0.00014633 -0.00027822 -0.00237929 -
0.00340790 -0.00626107 -0.20856912 0.13013402 -0.34788181 0.21109014 -0.12788184 0.35255066 </matrix>
</property>
<!--In QOOH: Vibrational frequencies (cm-1) were calculated from Hessian:
88.8083 154.742 223.916 265.268 271.806 292.618 334.839 364.111 406.443 455.145
492.787 584.044 791.587 892.303 931.074 958.574 995.228 1032.4 1050.18 1187.05
1287.25 1292.14 1400.85 1415.85 1423.38 1463.66 1485.15 1495.59 1503.11 1521.95
3068.23 3072.71 3142.83 3147.13 3151.43 3159.57 3159.87 3272.71 3834.78 -->
<property dictRef="me:frequenciesScaleFactor">
<scalar>0.9854</scalar>
</property>
<property dictRef="me:epsilon">
<scalar>443.08015</scalar>
</property>
<property dictRef="me:sigma">
<scalar>6.41</scalar>
</property>
<property title="Rotational Constants" dictRef="me:rotConsts">
<array units="cm-1">0.154 0.097 0.095 </array>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1 </scalar>
</property>
</propertyList>
<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D" UseSineTerms="yes">
<me:bondRef>b1</me:bondRef>
<me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
<me:PotentialPoint angle=" 0 " potential=" 0.246148502 "/>
<me:PotentialPoint angle=" 10 " potential=" 1.227531521 "/>
<me:PotentialPoint angle=" 20 " potential=" 2.985204002 "/>
<me:PotentialPoint angle=" 30 " potential=" 5.701730087 "/>
<me:PotentialPoint angle=" 40 " potential=" 9.355740831 "/>
<me:PotentialPoint angle=" 50 " potential=" 13.73452085 "/>
<me:PotentialPoint angle=" 60 " potential=" 18.45787149 "/>
<me:PotentialPoint angle=" 70 " potential=" 23.07023174 "/>
<me:PotentialPoint angle=" 80 " potential=" 27.18893498 "/>
<me:PotentialPoint angle=" 90 " potential=" 30.39401411 "/>
<me:PotentialPoint angle=" 100 " potential=" 32.20946597 "/>
<me:PotentialPoint angle=" 110 " potential=" 32.44082503 "/>
<me:PotentialPoint angle=" 120 " potential=" 31.05512026 "/>
<me:PotentialPoint angle=" 130 " potential=" 28.29306538 "/>

```
    <me:PotentialPoint  angle="  140      "          potential="       24.42205181      "/>
    <me:PotentialPoint  angle="  150      "          potential="       19.92597233      "/>
    <me:PotentialPoint  angle="  160      "          potential="       15.1789423       "/>
    <me:PotentialPoint  angle="  170      "          potential="       10.6172542       "/>
    <me:PotentialPoint  angle="  180      "          potential="       6.796852392      "/>
    <me:PotentialPoint  angle="  190      "          potential="       3.842742187      "/>
    <me:PotentialPoint  angle="  200      "          potential="       1.795280143      "/>
    <me:PotentialPoint  angle="  210      "          potential="       0.543533635      "/>
    <me:PotentialPoint  angle="  220      "          potential="       0.066900366      "/>
    <me:PotentialPoint  angle="  230      "          potential="       0.1967786        "/>
    <me:PotentialPoint  angle="  240      "          potential="       0.670019723      "/>
    <me:PotentialPoint  angle="  250      "          potential="       1.316908792      "/>
    <me:PotentialPoint  angle="  260      "          potential="       2.01850803       "/>
    <me:PotentialPoint  angle="  270      "          potential="       2.649557456      "/>
    <me:PotentialPoint  angle="  280      "          potential="       3.069448421      "/>
    <me:PotentialPoint  angle="  290      "          potential="       3.113365159      "/>
    <me:PotentialPoint  angle="  300      "          potential="       2.794679344      "/>
    <me:PotentialPoint  angle="  310      "          potential="       2.266709672      "/>
    <me:PotentialPoint  angle="  320      "          potential="       1.56611075       "/>
    <me:PotentialPoint  angle="  330      "          potential="       0.882532945      "/>
    <me:PotentialPoint  angle="  340      "          potential="       0.266635278      "/>
    <me:PotentialPoint  angle="  350      "          potential="       0          "/>
    <me:PotentialPoint  angle="  360      "          potential="       0.24600935       "/>
  </me:HinderedRotorPotential>
</me:ExtraDOSCMethod>
<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
  <me:bondRef>b3</me:bondRef>
  <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
    <me:PotentialPoint  angle="  0        "          potential="       0.319255549      "/>
    <me:PotentialPoint  angle="  10       "          potential="       0.019515341      "/>
    <me:PotentialPoint  angle="  20       "          potential="       1.207947917      "/>
    <me:PotentialPoint  angle="  30       "          potential="       3.780063625      "/>
    <me:PotentialPoint  angle="  40       "          potential="       7.229358884      "/>
    <me:PotentialPoint  angle="  50       "          potential="       10.66797886      "/>
    <me:PotentialPoint  angle="  60       "          potential="       12.97381898      "/>
    <me:PotentialPoint  angle="  70       "          potential="       13.3271719       "/>
    <me:PotentialPoint  angle="  80       "          potential="       11.56942591      "/>
    <me:PotentialPoint  angle="  90       "          potential="       8.580378172      "/>
    <me:PotentialPoint  angle="  100      "          potential="       5.061520291      "/>
    <me:PotentialPoint  angle="  110      "          potential="       2.114900636      "/>
    <me:PotentialPoint  angle="  120      "          potential="       0.351226263      "/>
    <me:PotentialPoint  angle="  130      "          potential="       0.060278855      "/>
    <me:PotentialPoint  angle="  140      "          potential="       1.175378589      "/>
```

```
    <me:PotentialPoint  angle="  150      "          potential="       3.601786924      "/>
    <me:PotentialPoint  angle="  160      "          potential="       7.141480773      "/>
    <me:PotentialPoint  angle="  170      "          potential="       10.45909145      "/>
    <me:PotentialPoint  angle="  180      "          potential="       12.90583954      "/>
    <me:PotentialPoint  angle="  190      "          potential="       13.17311806      "/>
    <me:PotentialPoint  angle="  200      "          potential="       11.66196165      "/>
    <me:PotentialPoint  angle="  210      "          potential="       8.754853149      "/>
    <me:PotentialPoint  angle="  220      "          potential="       5.201183763      "/>
    <me:PotentialPoint  angle="  230      "          potential="       2.253038694      "/>
    <me:PotentialPoint  angle="  240      "          potential="       0.41159701       "/>
    <me:PotentialPoint  angle="  250      "          potential="       0          "/>
    <me:PotentialPoint  angle="  260      "          potential="       1.2744177        "/>
    <me:PotentialPoint  angle="  270      "          potential="       3.78140263       "/>
    <me:PotentialPoint  angle="  280      "          potential="       7.236258698      "/>
    <me:PotentialPoint  angle="  290      "          potential="       10.65963502      "/>
    <me:PotentialPoint  angle="  300      "          potential="       13.02789116      "/>
    <me:PotentialPoint  angle="  310      "          potential="       13.29335284      "/>
    <me:PotentialPoint  angle="  320      "          potential="       11.56378108      "/>
    <me:PotentialPoint  angle="  330      "          potential="       8.562703306      "/>
    <me:PotentialPoint  angle="  340      "          potential="       5.191238369      "/>
    <me:PotentialPoint  angle="  350      "          potential="       2.270821205      "/>
    <me:PotentialPoint  angle="  360      "          potential="       0.319200414      "/>
  </me:HinderedRotorPotential>
  <me:periodicity>3</me:periodicity>
</me:ExtraDOSCMethod>
<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
  <me:bondRef>b4</me:bondRef>
  <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
    <me:PotentialPoint  angle="  0        "          potential="       0          "/>
    <me:PotentialPoint  angle="  10       "          potential="       0.097579333      "/>
    <me:PotentialPoint  angle="  20       "          potential="       0.386200548      "/>
    <me:PotentialPoint  angle="  30       "          potential="       0.846545216      "/>
    <me:PotentialPoint  angle="  40       "          potential="       1.398283539      "/>
    <me:PotentialPoint  angle="  50       "          potential="       1.835284887      "/>
    <me:PotentialPoint  angle="  60       "          potential="       2.166685999      "/>
    <me:PotentialPoint  angle="  70       "          potential="       2.459941221      "/>
    <me:PotentialPoint  angle="  80       "          potential="       2.691155879      "/>
    <me:PotentialPoint  angle="  90       "          potential="       2.654243974      "/>
    <me:PotentialPoint  angle="  100      "          potential="       2.405097152      "/>
    <me:PotentialPoint  angle="  110      "          potential="       1.947887331      "/>
    <me:PotentialPoint  angle="  120      "          potential="       1.502796818      "/>
    <me:PotentialPoint  angle="  130      "          potential="       1.160255709      "/>
    <me:PotentialPoint  angle="  140      "          potential="       0.79563152       "/>
```

```
    <me:PotentialPoint  angle="  150      "        potential="       0.310221204     "/>
    <me:PotentialPoint  angle="  160      "        potential="       0.063497718     "/>
    <me:PotentialPoint  angle="  170      "        potential="       0.006742284     "/>
    <me:PotentialPoint  angle="  180      "        potential="       0.135181744     "/>
    <me:PotentialPoint  angle="  190      "        potential="       0.399167893     "/>
    <me:PotentialPoint  angle="  200      "        potential="       0.734609649     "/>
    <me:PotentialPoint  angle="  210      "        potential="       1.079440194     "/>
    <me:PotentialPoint  angle="  220      "        potential="       1.397855583     "/>
    <me:PotentialPoint  angle="  230      "        potential="       1.695763191     "/>
    <me:PotentialPoint  angle="  240      "        potential="       1.889147019     "/>
    <me:PotentialPoint  angle="  250      "        potential="       2.184560403     "/>
    <me:PotentialPoint  angle="  260      "        potential="       2.557777853     "/>
    <me:PotentialPoint  angle="  270      "        potential="       2.446732331     "/>
    <me:PotentialPoint  angle="  280      "        potential="       1.873630314     "/>
    <me:PotentialPoint  angle="  290      "        potential="       1.424178845     "/>
    <me:PotentialPoint  angle="  300      "        potential="       1.219342586     "/>
    <me:PotentialPoint  angle="  310      "        potential="       1.061158837     "/>
    <me:PotentialPoint  angle="  320      "        potential="       0.849939988     "/>
    <me:PotentialPoint  angle="  330      "        potential="       0.532881982     "/>
    <me:PotentialPoint  angle="  340      "        potential="       0.287870322     "/>
    <me:PotentialPoint  angle="  350      "        potential="       0.077470629     "/>
    <me:PotentialPoint  angle="  360      "        potential="       0.000152279     "/>
  </me:HinderedRotorPotential>
  <me:periodicity>2</me:periodicity>
</me:ExtraDOSCMethod>
<me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
  <me:bondRef>b5</me:bondRef>
  <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
    <me:PotentialPoint  angle="  0        "        potential="       3.341465974     "/>
    <me:PotentialPoint  angle="  10       "        potential="       4.735693115     "/>
    <me:PotentialPoint  angle="  20       "        potential="       8.446343771     "/>
    <me:PotentialPoint  angle="  30       "        potential="       13.78238372     "/>
    <me:PotentialPoint  angle="  40       "        potential="       19.25901394     "/>
    <me:PotentialPoint  angle="  50       "        potential="       23.45074283     "/>
    <me:PotentialPoint  angle="  60       "        potential="       25.18996067     "/>
    <me:PotentialPoint  angle="  70       "        potential="       23.87492124     "/>
    <me:PotentialPoint  angle="  80       "        potential="       19.94848074     "/>
    <me:PotentialPoint  angle="  90       "        potential="       14.33950957     "/>
    <me:PotentialPoint  angle="  100      "        potential="       8.663890076     "/>
    <me:PotentialPoint  angle="  110      "        potential="       4.325868318     "/>
    <me:PotentialPoint  angle="  120      "        potential="       2.63988774      "/>
    <me:PotentialPoint  angle="  130      "        potential="       4.02019448      "/>
    <me:PotentialPoint  angle="  140      "        potential="       8.011109385     "/>
```

```
    <me:PotentialPoint  angle="  150      "        potential="      13.5839458      "/>
    <me:PotentialPoint  angle="  160      "        potential="      19.15079083     "/>
    <me:PotentialPoint  angle="  170      "        potential="      22.93285771     "/>
    <me:PotentialPoint  angle="  180      "        potential="      23.9527043      "/>
    <me:PotentialPoint  angle="  190      "        potential="      21.7116799      "/>
    <me:PotentialPoint  angle="  200      "        potential="      16.85295848     "/>
    <me:PotentialPoint  angle="  210      "        potential="      10.60405056     "/>
    <me:PotentialPoint  angle="  220      "        potential="      4.607463695     "/>
    <me:PotentialPoint  angle="  230      "        potential="      0.675871963     "/>
    <me:PotentialPoint  angle="  240      "        potential="      0          "/>
    <me:PotentialPoint  angle="  250      "        potential="      2.565047863     "/>
    <me:PotentialPoint  angle="  260      "        potential="      7.461655247     "/>
    <me:PotentialPoint  angle="  270      "        potential="      13.30121883     "/>
    <me:PotentialPoint  angle="  280      "        potential="      18.65571079     "/>
    <me:PotentialPoint  angle="  290      "        potential="      22.34759963     "/>
    <me:PotentialPoint  angle="  300      "        potential="      23.73979463     "/>
    <me:PotentialPoint  angle="  310      "        potential="      22.5388673      "/>
    <me:PotentialPoint  angle="  320      "        potential="      19.1658717      "/>
    <me:PotentialPoint  angle="  330      "        potential="      14.22379328     "/>
    <me:PotentialPoint  angle="  340      "        potential="      8.950497532     "/>
    <me:PotentialPoint  angle="  350      "        potential="      4.914421402     "/>
    <me:PotentialPoint  angle="  360      "        potential="      3.341463348     "/>
   </me:HinderedRotorPotential>
   <me:periodicity>3</me:periodicity>
  </me:ExtraDOSCMethod>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
   <me:deltaEDown bathGas="He" units="cm-1" lower="10" upper="350" stepsize="0.10" >150</me:deltaEDown>
   <!--<me:deltaEDownTExponent bathGas="He" referenceTemperature="298" >1.0</me:deltaEDownTExponent>-->
   <me:deltaEDown bathGas="N2" units="cm-1" lower="10" upper="350" stepsize="0.10">250</me:deltaEDown>
                <!--<me:deltaEDownTExponent bathGas="N2" referenceTemperature="298">0.25</me:deltaEDownTExponent>-->
  </me:energyTransferModel>
  <me:DOSCMethod>QMRotors</me:DOSCMethod>
</molecule>
<molecule xmlns="http://www.xml-cml.org/schema" id="TS">
  <atomArray>
   <atom id="a1" elementType="C" x3="0.092035" y3="0.059638" z3="-0.023566"/>
   <atom id="a2" elementType="H" x3="0.108051" y3="0.055720" z3="1.066403"/>
   <atom id="a3" elementType="H" x3="1.112650" y3="0.151914" z3="-0.394152"/>
   <atom id="a4" elementType="H" x3="-0.325585" y3="-0.879557" z3="-0.378191"/>
   <atom id="a5" elementType="C" x3="-0.748574" y3="1.238108" z3="-0.521472"/>
   <atom id="a6" elementType="C" x3="-0.212165" y3="2.557200" z3="0.035324"/>
   <atom id="a7" elementType="H" x3="0.796943" y3="2.723993" z3="-0.338702"/>
   <atom id="a8" elementType="H" x3="-0.845131" y3="3.385016" z3="-0.279902"/>
```

```
  <atom id="a9" elementType="H" x3="-0.185582" y3="2.519518" z3="1.123751"/>
  <atom id="a10" elementType="C" spinMultiplicity="2" x3="-0.811967" y3="1.276109" z3="-2.012558"/>
  <atom id="a11" elementType="H" x3="0.092672" y3="1.435377" z3="-2.579225"/>
  <atom id="a12" elementType="H" x3="-1.724174" y3="1.045284" z3="-2.537436"/>
  <atom id="a13" elementType="O" x3="-2.063843" y3="1.172607" z3="0.045066"/>
  <atom id="a14" elementType="O" x3="-2.674915" y3="-0.047634" z3="-0.349570"/>
  <atom id="a15" elementType="H" x3="-3.382762" y3="0.268286" z3="-0.921121"/>
</atomArray>
<bondArray>
  <bond atomRefs2="a12 a10" order="1"/>
  <bond atomRefs2="a11 a10" order="1"/>
  <bond id ="b4" atomRefs2="a10 a5" order="1"/>
  <bond atomRefs2="a15 a14" order="1"/>
  <bond id ="b3" atomRefs2="a5 a1" order="1"/>
  <bond id="b5" atomRefs2="a5 a6" order="1"/>
  <bond id="b2" atomRefs2="a5 a13" order="1"/>
  <bond atomRefs2="a3 a1" order="1"/>
  <bond atomRefs2="a8 a6" order="1"/>
  <bond atomRefs2="a7 a6" order="1"/>
  <bond atomRefs2="a4 a1" order="1"/>
  <bond id="b1" atomRefs2="a14 a13" order="1"/>
  <bond atomRefs2="a1 a2" order="1"/>
  <bond atomRefs2="a6 a9" order="1"/>
</bondArray>
<propertyList>
  <property title="program">
    <scalar>Gaussian 09, Revision D.01</scalar>
  </property>
  <property title="basis">
    <scalar>6-311+G(3d,2p) (5D, 7F)</scalar>
  </property>
  <property title="File Format">
    <scalar>g03</scalar>
  </property>
  <property title="Energy" dictRef="me:ZPE">
    <scalar units="kJ/mol" lower="30" upper="60" stepsize="0.5" >42</scalar>
                  <!--  <scalar units="kJ/mol"  >48</scalar> -->
  </property>
  <property title="Rotational Constants" dictRef="me:rotConsts">
    <array units="cm-1">0.157 0.096 0.094 </array>
  </property>
   <property title="Hessian" dictRef="me:hessian">
```

<matrix rows="45" matrixType="squareSymmetricLT" units="Hartree/Bohr2">0.56892269 0.04311154 0.52781377 -0.01358660 0.03064768 0.57100920 -0.04630081 -0.00099514
0.00176989 0.04665187 -0.00053900 -0.04788103 -0.00393312 -0.00121544 0.05091863 -0.00028798 -0.00207285 -0.32035825 0.00039914 0.00092457 0.34755874 -0.28701157
0.00006439 0.08394558 0.00173547 -0.00014670 -0.00037512 0.31240751 -0.00213616 -0.04932388 0.00100325 0.00007552 -0.00150834 -0.00019684 -0.00028909 0.04923894
0.08463572 0.00023241 -0.07578118 0.03140341 -0.00000346 -0.00795902 -0.09222266 -0.00143311 0.07789583 -0.10711879 -0.10683616 -0.04160337 -0.00050107 0.00122433
0.00039063 -0.01213460 -0.02469507 -0.01085881 0.11186904 -0.10304439 -0.23094030 -0.07172179 0.00099103 0.00069400 0.00028409 0.00103157 0.00173495 0.00138020 0.11322712
0.25294302 -0.04192034 -0.07356505 -0.07602353 -0.01568837 -0.02712098 -0.00833404 0.00453282 0.01038778 0.00285949 0.04666128 0.07755880 0.07885127 -0.09477478
0.04706497 -0.02630718 -0.00137760 -0.00037724 -0.00091027 -0.01368067 0.02259467 -0.01128436 0.00607516 -0.01488820 0.00624572 0.49701009 0.04116425 -0.17243902
0.03588337 -0.00038177 -0.00023142 -0.00007148 -0.00400399 0.00322788 -0.00144968 0.01454267 -0.02451727 0.01029630 -0.00054624 0.53881320 -0.01836675 0.03597324 -
0.09473605 -0.01736874 0.02957372 -0.01248735 0.00627772 -0.01178796 0.00264163 0.00572295 -0.00945608 0.00178063 0.12374713 0.00472702 0.50035810 0.01094808 0.01267404
0.00434188 -0.00011528 -0.00020674 0.00012832 0.00000747 -0.00052218 0.00028768 -0.00149285 0.00416925 -0.00121606 -0.08820430 -0.03399378 -0.01398494 0.57379941 -
0.00896205 -0.02992233 -0.00802602 -0.00071272 0.00138872 -0.00062760 -0.00071132 0.00058733 -0.00018476 0.00233368 -0.00302892 0.00165607 -0.04018292 -0.18127847 -
0.03437917 -0.03882421 0.51633789 0.00381503 0.00956513 0.00482818 0.00018837 0.00065749 0.00034931 0.00019288 -0.00020361 -0.00003777 -0.00097180 0.00273737 -0.00042332
-0.02136160 -0.03444658 -0.09222738 -0.00914085 -0.02879244 0.57486462 -0.00010942 0.00063847 0.00011293 0.00000493 0.00000609 -0.00009297 0.00068895 -0.00005448 -
0.00003207 0.00024597 -0.00003016 -0.00025534 -0.01200835 0.00268873 0.00532832 -0.28229138 -0.01861099 0.08839470 0.30680677 0.00046598 0.00071265 0.00020700 -0.00002869
-0.00004758 0.00002620 0.00022553 -0.00095451 -0.00002938 0.00018640 0.00031021 -0.00016964 -0.02411869 0.00183037 0.01270070 -0.01645567 -0.05027340 0.00613523
0.02071490 0.05080903 0.00030247 0.00018075 -0.00010799 0.00016748 0.00001045 -0.00002653 -0.00005978 0.00007689 0.00030520 -0.00013847 0.00011699 -0.00006827 -0.01051246
0.00033875 0.00245138 0.08895387 0.00695406 -0.07938431 -0.09703052 -0.00647112 0.08210692 -0.00090199 -0.00214928 -0.00062065 -0.00012215 0.00002890 -0.00009710
0.00027305 -0.00019494 -0.00011259 0.00064497 -0.00061742 0.00006856 0.00567667 -0.01172065 0.00504661 -0.12695605 0.11430969 -0.05016184 -0.01433096 0.02293234 -
0.01126106 0.13382539 -0.00409613 -0.00379301 -0.00282575 -0.00008789 0.00025557 -0.00004599 0.00000936 0.00032789 -0.00013809 0.00084574 -0.00154992 0.00059648
0.01820194 -0.02420765 0.01060610 0.11094873 -0.20540805 0.06976988 -0.00216741 0.00307990 -0.00218713 -0.12237021 0.22559450 -0.00086902 -0.00157284 -0.00023545
0.00000538 -0.00032990 0.00030944 -0.00026822 0.00012163 -0.00007903 0.00008484 -0.00047284 0.00068946 0.00648226 -0.00846774 0.00150654 -0.05091986 0.07172559 -
0.07938781 0.00580765 -0.01030935 0.00340644 0.05605057 -0.07587619 0.08207242 -0.00015504 0.00060255 0.00020349 0.00036950 0.00004808 0.00014617 -0.00001909 0.00003602
0.00018207 -0.00014122 0.00005829 -0.00000427 -0.00142311 -0.00005527 -0.01468180 -0.04613599 0.00148108 -0.00438031 0.00230333 0.00119130 0.03102702 -0.00066723 -
0.00174481 -0.01814553 0.04632883 0.00005210 0.00147974 -0.00065725 -0.00000087 -0.00068522 0.00039699 0.00001921 -0.00004391 0.00001973 -0.00006973 0.00026902 0.00031885
-0.00026213 -0.00100185 -0.03135860 0.00114261 -0.04783983 -0.00472059 0.00043940 -0.00135291 0.00245859 -0.00092234 0.00133370 0.02527557 0.00040633 0.05122940
0.00010283 0.00061904 0.00036782 0.00015986 -0.00033220 0.00042635 -0.00008436 -0.00006354 -0.00004256 -0.00010028 0.00004177 0.00028542 -0.00112940 -0.00032376 -
0.01104550 -0.00613266 -0.00691554 -0.32052276 -0.00058221 -0.00010059 -0.00868213 0.00028968 -0.00054287 -0.00860577 0.00623044 0.00864908 0.34774656 -0.00158764
0.00241878 -0.01603834 -0.00126729 0.00181645 -0.00035825 0.00051685 -0.00089155 0.00052758 0.00027059 -0.00087094 0.00079997 -0.03524818 0.00018598 -0.07008863 -
0.00136189 -0.00301342 -0.01364912 0.00044421 0.00082029 0.00034407 0.00019151 0.00087869 0.00087219 -0.00090970 -0.00151607 -0.00019726 0.10986619 0.00162719 -0.00124203
0.03015301 0.00333194 -0.00448963 0.00204374 -0.00034501 0.00096088 -0.00089161 0.00028885 0.00043584 0.00114530 -0.00143727 -0.07870532 -0.00391485 -0.00191337 -
0.00291605 -0.03211120 0.00036083 0.00117516 0.00086022 -0.00030041 0.00043267 -0.00109023 -0.00294404 -0.00506929 -0.00207388 -0.01607256 0.67177511 -0.00451504
0.00276428 -0.01646170 -0.00118823 0.00133563 0.00042871 -0.00041636 -0.00017271 0.00058781 0.00079397 -0.00106384 0.00071338 -0.12139204 -0.00681068 -0.22775766 -
0.00439621 -0.00362834 -0.01524558 -0.00041300 0.00014672 0.00057554 0.00069674 0.00118509 0.00064069 -0.00075778 -0.00118389 0.00039766 0.21603939 0.00362898 0.44042207
0.00026780 -0.00065552 -0.00362817 -0.00063207 0.00091376 -0.00050918 -0.00008572 0.00000053 0.00008225 0.00005487 -0.00008303 0.00008712 -0.00259707 0.01441674
0.00052978 0.00024255 0.00088207 0.00123232 -0.00025751 -0.00002820 -0.00009308 0.00020456 -0.00051154 -0.00017433 0.00011442 -0.00007656 0.00025975 -0.04394671
0.06346885 -0.05143125 0.03810836 -0.00032240 0.00038157 -0.00041535 0.00010020 0.00036476 -0.00005258 0.00000002 -0.00001388 0.00001708 0.00002288 0.00034252 -0.00016700
-0.00039311 0.00350235 -0.00331866 -0.00052161 0.00115256 -0.00020758 -0.00010882 -0.00002658 0.00012894 0.00023733 0.00018129 -0.00011056 0.00000450 0.00002780
0.00003635 0.06187467 -0.27773363 0.11836391 -0.06692149 0.28272835 0.00071976 -0.00154020 -0.00354714 -0.00064421 0.00108907 -0.00017254 -0.00004850 -0.00000396
0.00010787 0.00008129 0.00017435 0.00004128 -0.00423513 0.01959496 -0.00818458 -0.00006961 0.00141084 0.00123174 -0.00009883 -0.00020270 -0.00007982 0.00008319 -
0.00088602 -0.00029706 0.00024643 -0.00020121 0.00013028 -0.04205700 0.11593943 -0.11341962 0.04791561 -0.12642853 0.11630573 0.00027308 -0.00088778 0.00129114 0.00011833
0.00009088 0.00025749 -0.00025206 0.00001403 -0.00009221 0.00017781 0.00051274 -0.00019922 -0.00104564 -0.01473689 0.00052683 0.00019137 0.00050093 -0.00355291 -
0.00008307 -0.00000453 0.00008404 0.00006408 0.00005062 0.00006548 -0.00048869 -0.00099250 -0.00048258 -0.03647392 -0.04781036 -0.04146590 0.00462524 0.00661862
0.00201187 0.03011555 0.00042058 0.00110472 0.00022061 -0.00000198 0.00002723 -0.00001746 0.00009134 -0.00002070 -0.00011524 -0.00023768 0.00020644 0.00005814 0.00001651

0.00207353 0.00291225 0.00030700 0.00049055 0.00000035 0.00000390 -0.00001786 0.00000099 -0.00004787 0.00034444 0.00016486 -0.00019362 0.00025479 0.00002177 -0.04596614 -0.29382753 -0.11647285 -0.00528805 -0.01184631 -0.01150691 0.05038088 0.29992156 0.00003548 -0.00138109 0.00127381 0.00021594 0.00022897 0.00011817 -0.00009847 0.00019097 -0.00007880 -0.00001627 0.00086139 -0.00033235 -0.00308817 -0.02011084 -0.00736569 0.00055353 0.00148495 -0.00364047 -0.00004073 0.00001512 0.00010320 0.00011127 -0.00019837 0.00004399 -0.00052469 -0.00117366 -0.00015506 -0.03251308 -0.11353392 -0.10643199 0.00134189 0.01244101 0.01035318 0.03738035 0.12416429 0.10857921 -0.04292338 0.00451621 0.01098272 0.00199953 -0.00168256 0.00035676 -0.00301686 0.00643229 -0.00316511 0.00217250 -0.00066728 0.00063426 -0.26321893 -0.00888278 -0.03678036 -0.03836985 -0.00807696 0.01069670 -0.00198557 -0.00617446 -0.00269290 0.00214969 0.00045698 0.00050951 0.00174799 0.00173405 0.00024825 0.02539991 0.00214573 -0.01426875 0.00406474 -0.00081443 -0.00449833 0.00296415 0.00075644 -0.00381884 0.32530417 0.03181664 0.00479071 -0.00971537 -0.00096529 0.00120757 0.00005288 0.00430700 -0.00441881 0.00301227 -0.00071658 0.00319043 -0.00118563 -0.00418992 -0.06699854 -0.00135190 -0.03543739 0.00138780 0.01117674 -0.00406662 -0.00541143 -0.00328829 0.00063377 0.00354505 0.00110900 0.00083300 0.00141849 -0.00020532 -0.00208007 -0.01292130 0.00582985 -0.00600252 0.00095143 0.00313297 0.00608024 0.00120163 -0.00355263 0.00448185 0.08466541 -0.00682376 0.00081405 0.00824995 -0.00097572 -0.00140085 -0.00053798 0.00016745 0.00116238 -0.00028915 -0.00066262 -0.00046464 0.00043091 0.08227116 0.00076720 -0.02123514 -0.00503944 -0.00080560 0.00780661 0.00048397 -0.00094821 -0.00041012 -0.00071686 0.00031199 0.00047981 -0.00118905 0.00126471 -0.00073283 -0.13114639 -0.00111459 0.15177047 0.00311872 0.00126932 -0.00229289 0.00327897 -0.00119833 -0.00221285 0.10744293 -0.00019066 -0.34029943 0.00065935 0.00051714 -0.00085004 -0.00088109 0.00023512 0.00069689 0.00053583 -0.00038431 0.00043652 -0.00010603 0.00024865 0.00024374 0.00618326 0.00006901 0.02353574 -0.00052228 -0.00053159 -0.00181596 0.00044229 0.00044486 0.00117709 0.00002903 -0.00015390 0.00018245 -0.00037149 -0.00024917 0.00163002 -0.01541527 0.00022520 0.02185078 -0.00018946 0.00020669 0.00046036 -0.00025109 -0.00024052 0.00055122 -0.01644164 0.00439121 -0.04441068 0.22943324 0.00067400 -0.00050623 -0.00084628 0.00005238 -0.00005903 -0.00044574 -0.00017626 0.00008242 -0.00031055 -0.00011885 -0.00003874 0.00006209 -0.00148374 -0.00080541 -0.00307046 -0.00127737 -0.00094373 0.00060304 0.00013730 0.00040188 0.00091679 0.00020236 0.00007397 -0.00049783 0.00054724 -0.00007747 0.00142932 0.00284209 0.00198512 -0.00277353 -0.00024297 -0.00006241 -0.00054557 0.00011867 0.00014942 0.00063346 0.00770821 -0.01371277 -0.00445289 -0.26706437 0.34895584 -0.00247562 -0.00085991 0.00205797 0.00165129 -0.00082155 0.00034336 -0.00141843 0.00083161 -0.00025274 0.00058251 0.00004027 -0.00049068 -0.01883776 0.00033965 -0.02874984 -0.00331471 0.00056740 0.00094192 -0.00144866 -0.00099157 -0.00010887 0.00055232 0.00002662 -0.00044001 0.00156140 0.00067984 0.00035973 0.08577898 0.00144604 -0.11485660 0.00151179 -0.00157485 -0.00006630 0.00078777 0.00172825 -0.00028683 -0.08173383 0.01088016 0.20720214 0.01806396 -0.02007397 -0.04285189 -0.00018758 -0.00008422 -0.00001327 0.00031770 -0.00019593 0.00025546 0.00003543 0.00001471 0.00021256 -0.00001635 -0.00003723 0.00001012 -0.00136653 0.00125400 0.00055613 0.00026099 0.00011872 0.00051440 0.00012979 -0.00017137 -0.00026776 -0.00008058 -0.00026017 0.00031663 -0.00055248 0.00029567 -0.00021207 -0.00047865 -0.00062558 0.00086368 0.00002598 0.00001697 0.00013310 0.00006487 -0.00000080 -0.00008946 0.00015355 0.00091467 -0.00579866 -0.20310465 0.25808132 -0.00126100 0.20479852 -0.00023215 -0.00023533 0.00002600 -0.00016128 0.00004577 -0.00019794 -0.00007605 0.00012372 -0.00010582 0.00000240 -0.00005127 0.00012848 0.00000137 0.00073761 0.00214465 -0.00008930 0.00026593 -0.00016324 0.00004885 -0.00023492 -0.00009688 -0.00002127 -0.00021035 0.00033085 -0.00027065 0.00005754 -0.00023963 -0.00042619 0.00013998 -0.00114862 0.00012791 0.00005018 -0.00002652 0.00006444 -0.00006191 -0.00006964 -0.00193331 0.00110432 0.00498612 0.26228597 -0.33544284 0.00778202 -0.25932075 0.33371156 -0.00076619 0.00019537 -0.00053564 -0.00009550 0.00012218 0.00034164 -0.00012455 0.00008721 0.00012244 0.00003415 -0.00001606 0.00002037 0.00031211 -0.00026650 -0.00494909 -0.00005095 -0.00043945 0.00084702 -0.00013325 -0.00000839 -0.00008064 0.00007118 0.00020426 -0.00010364 0.00008640 0.00023184 0.00007280 0.00168590 -0.00048645 -0.00136317 -0.00024323 0.00001851 -0.00011013 0.00010887 0.00003929 0.00003247 0.01608700 -0.01570406 -0.00792949 -0.02175208 0.02937211 -0.02280136 0.00478014 -0.01334986 0.03643641 </matrix>
</property>
<!-- In TS: Vibrational frequencies (cm-1) were calculated from Hessian:
104.62 183.895 196.19 209.193 250.495 337.272 353.434 397.798 422.924 470.314
569.191 771.044 785.009 912.064 922.631 960.874 1007.44 1030.86 1054.27 1179.01
1287.69 1357.22 1409.58 1419.11 1473.34 1480.06 1497.3 1511.52 1518.7 3067.38
3071.85 3142.02 3147.34 3153.15 3155.78 3174.41 3297.01 3862.64 -->
<property dictRef="me:frequenciesScaleFactor">
<scalar>0.9854</scalar>
</property>
<property title="Symmetry Number" dictRef="me:symmetryNumber">
<scalar>1 </scalar>
</property>
</propertyList>

```
    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D" UseSineTerms="yes">
      <me:bondRef>b1</me:bondRef>
      <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
<me:PotentialPoint        angle="  0       "        potential="      0.371539756     "/>
<me:PotentialPoint        angle="  10      "        potential="      0.064729077     "/>
<me:PotentialPoint        angle="  20      "        potential="      0         "/>
<me:PotentialPoint        angle="  30      "        potential="      0.044533731     "/>
<me:PotentialPoint        angle="  40      "        potential="      0.19082134      "/>
<me:PotentialPoint        angle="  50      "        potential="      0.296492464     "/>
<me:PotentialPoint        angle="  60      "        potential="      0.293011051     "/>
<me:PotentialPoint        angle="  70      "        potential="      0.177047967     "/>
<me:PotentialPoint        angle="  80      "        potential="      0.055482066     "/>
<me:PotentialPoint        angle="  90      "        potential="      0.025997701     "/>
<me:PotentialPoint        angle="  100     "        potential="      0.063474088     "/>
<me:PotentialPoint        angle="  110     "        potential="      0.393436426     "/>
<me:PotentialPoint        angle="  120     "        potential="      1.048351648     "/>
<me:PotentialPoint        angle="  130     "        potential="      2.174097785     "/>
<me:PotentialPoint        angle="  140     "        potential="      3.768973513     "/>
<me:PotentialPoint        angle="  150     "        potential="      5.858312281     "/>
<me:PotentialPoint        angle="  160     "        potential="      8.426271823     "/>
<me:PotentialPoint        angle="  170     "        potential="      11.43634719     "/>
<me:PotentialPoint        angle="  180     "        potential="      14.76286619     "/>
<me:PotentialPoint        angle="  190     "        potential="      18.11007676     "/>
<me:PotentialPoint        angle="  200     "        potential="      21.24658832     "/>
<me:PotentialPoint        angle="  210     "        potential="      23.93764706     "/>
<me:PotentialPoint        angle="  220     "        potential="      26.0067406      "/>
<me:PotentialPoint        angle="  230     "        potential="      27.1236703      "/>
<me:PotentialPoint        angle="  240     "        potential="      27.10397905     "/>
<me:PotentialPoint        angle="  250     "        potential="      25.96191806     "/>
<me:PotentialPoint        angle="  260     "        potential="      23.92992546     "/>
<me:PotentialPoint        angle="  270     "        potential="      21.27001829     "/>
<me:PotentialPoint        angle="  280     "        potential="      18.13713779     "/>
<me:PotentialPoint        angle="  290     "        potential="      14.77860081     "/>
<me:PotentialPoint        angle="  300     "        potential="      11.48061049     "/>
<me:PotentialPoint        angle="  310     "        potential="      8.457594039     "/>
<me:PotentialPoint        angle="  320     "        potential="      5.840112315     "/>
<me:PotentialPoint        angle="  330     "        potential="      3.71723541      "/>
<me:PotentialPoint        angle="  340     "        potential="      2.11053443      "/>
<me:PotentialPoint        angle="  350     "        potential="      1.013185701     "/>
<me:PotentialPoint        angle="  360     "        potential="      0.371629023     "/>
      </me:HinderedRotorPotential>
    </me:ExtraDOSCMethod>
    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
```

```
      <me:bondRef>b3</me:bondRef>
      <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
<me:PotentialPoint        angle="  0      "        potential="      0          "/>
<me:PotentialPoint        angle="  10     "        potential="      0.833766908      "/>
<me:PotentialPoint        angle="  20     "        potential="      2.937194109      "/>
<me:PotentialPoint        angle="  30     "        potential="      5.925771879      "/>
<me:PotentialPoint        angle="  40     "        potential="      9.132132248      "/>
<me:PotentialPoint        angle="  50     "        potential="      11.26651935      "/>
<me:PotentialPoint        angle="  60     "        potential="      11.93061594      "/>
<me:PotentialPoint        angle="  70     "        potential="      10.72073041      "/>
<me:PotentialPoint        angle="  80     "        potential="      8.171810989      "/>
<me:PotentialPoint        angle="  90     "        potential="      5.071599585      "/>
<me:PotentialPoint        angle="  100    "        potential="      2.339352006      "/>
<me:PotentialPoint        angle="  110    "        potential="      0.528400254      "/>
<me:PotentialPoint        angle="  120    "        potential="      0.019578354      "/>
<me:PotentialPoint        angle="  130    "        potential="      0.891349374      "/>
<me:PotentialPoint        angle="  140    "        potential="      2.943096233      "/>
<me:PotentialPoint        angle="  150    "        potential="      5.811271198      "/>
<me:PotentialPoint        angle="  160    "        potential="      8.854661531      "/>
<me:PotentialPoint        angle="  170    "        potential="      11.13513933      "/>
<me:PotentialPoint        angle="  180    "        potential="      11.94941977      "/>
<me:PotentialPoint        angle="  190    "        potential="      10.97639372      "/>
<me:PotentialPoint        angle="  200    "        potential="      8.62794173       "/>
<me:PotentialPoint        angle="  210    "        potential="      5.576493737      "/>
<me:PotentialPoint        angle="  220    "        potential="      2.708615454      "/>
<me:PotentialPoint        angle="  230    "        potential="      0.705369456      "/>
<me:PotentialPoint        angle="  240    "        potential="      0.019993183      "/>
<me:PotentialPoint        angle="  250    "        potential="      0.769237369      "/>
<me:PotentialPoint        angle="  260    "        potential="      2.811928879      "/>
<me:PotentialPoint        angle="  270    "        potential="      5.682065092      "/>
<me:PotentialPoint        angle="  280    "        potential="      8.767668214      "/>
<me:PotentialPoint        angle="  290    "        potential="      11.09779946      "/>
<me:PotentialPoint        angle="  300    "        potential="      11.94987136      "/>
<me:PotentialPoint        angle="  310    "        potential="      10.94370099      "/>
<me:PotentialPoint        angle="  320    "        potential="      8.486387897      "/>
<me:PotentialPoint        angle="  330    "        potential="      5.339250932      "/>
<me:PotentialPoint        angle="  340    "        potential="      2.466694007      "/>
<me:PotentialPoint        angle="  350    "        potential="      0.552363192      "/>
<me:PotentialPoint        angle="  360    "        potential="      0.020281988      "/>

      </me:HinderedRotorPotential>
      <me:periodicity>3</me:periodicity>
    </me:ExtraDOSCMethod>
```

```
    <me:ExtraDOSCMethod xsi:type="me:HinderedRotorQM1D">
      <me:bondRef>b5</me:bondRef>
      <me:HinderedRotorPotential format="numerical" units="kJ/mol" expansionSize="7">
<me:PotentialPoint angle="  0  "  potential="  0  "/>
<me:PotentialPoint angle="  10  "  potential="  0.833766908  "/>
<me:PotentialPoint angle="  20  "  potential="  2.937194109  "/>
<me:PotentialPoint angle="  30  "  potential="  5.925771879  "/>
<me:PotentialPoint angle="  40  "  potential="  9.132132248  "/>
<me:PotentialPoint angle="  50  "  potential="  11.26651935  "/>
<me:PotentialPoint angle="  60  "  potential="  11.93061594  "/>
<me:PotentialPoint angle="  70  "  potential="  10.72073041  "/>
<me:PotentialPoint angle="  80  "  potential="  8.171810989  "/>
<me:PotentialPoint angle="  90  "  potential="  5.071599585  "/>
<me:PotentialPoint angle="  100  "  potential="  2.339352006  "/>
<me:PotentialPoint angle="  110  "  potential="  0.528400254  "/>
<me:PotentialPoint angle="  120  "  potential="  0.019578354  "/>
<me:PotentialPoint angle="  130  "  potential="  0.891349374  "/>
<me:PotentialPoint angle="  140  "  potential="  2.943096233  "/>
<me:PotentialPoint angle="  150  "  potential="  5.811271198  "/>
<me:PotentialPoint angle="  160  "  potential="  8.854661531  "/>
<me:PotentialPoint angle="  170  "  potential="  11.13513933  "/>
<me:PotentialPoint angle="  180  "  potential="  11.94941977  "/>
<me:PotentialPoint angle="  190  "  potential="  10.97639372  "/>
<me:PotentialPoint angle="  200  "  potential="  8.62794173  "/>
<me:PotentialPoint angle="  210  "  potential="  5.576493737  "/>
<me:PotentialPoint angle="  220  "  potential="  2.708615454  "/>
<me:PotentialPoint angle="  230  "  potential="  0.705369456  "/>
<me:PotentialPoint angle="  240  "  potential="  0.019993183  "/>
<me:PotentialPoint angle="  250  "  potential="  0.769237369  "/>
<me:PotentialPoint angle="  260  "  potential="  2.811928879  "/>
<me:PotentialPoint angle="  270  "  potential="  5.682065092  "/>
<me:PotentialPoint angle="  280  "  potential="  8.767668214  "/>
<me:PotentialPoint angle="  290  "  potential="  11.09779946  "/>
<me:PotentialPoint angle="  300  "  potential="  11.94987136  "/>
<me:PotentialPoint angle="  310  "  potential="  10.94370099  "/>
<me:PotentialPoint angle="  320  "  potential="  8.486387897  "/>
<me:PotentialPoint angle="  330  "  potential="  5.339250932  "/>
<me:PotentialPoint angle="  340  "  potential="  2.466694007  "/>
<me:PotentialPoint angle="  350  "  potential="  0.552363192  "/>
<me:PotentialPoint angle="  360  "  potential="  0.020281988  "/>
      </me:HinderedRotorPotential>
      <me:periodicity>3</me:periodicity>
    </me:ExtraDOSCMethod>
```

```
  <me:DOSCMethod>QMRotors</me:DOSCMethod>
</molecule>
<molecule id="DMO">
  <atomArray>
    <atom id="a1" elementType="C" x3="0.129803" y3="0.000001" z3="-0.053098"/>
    <atom id="a2" elementType="C" x3="0.928938" y3="-1.278625" z3="-0.051980"/>
    <atom id="a3" elementType="H" x3="1.553069" y3="-1.341460" z3="-0.946608"/>
    <atom id="a4" elementType="H" x3="0.266503" y3="-2.144281" z3="-0.020319"/>
    <atom id="a5" elementType="H" x3="1.581949" y3="-1.309964" z3="0.824010"/>
    <atom id="a6" elementType="C" x3="0.928849" y3="1.278685" z3="-0.051957"/>
    <atom id="a7" elementType="H" x3="0.266335" y3="2.144265" z3="-0.019880"/>
    <atom id="a8" elementType="H" x3="1.552656" y3="1.341774" z3="-0.946793"/>
    <atom id="a9" elementType="H" x3="1.582164" y3="1.309903" z3="0.823809"/>
    <atom id="a10" elementType="C" x3="-1.244504" y3="-0.000017" z3="-0.573820"/>
    <atom id="a11" elementType="H" x3="-1.667749" y3="0.920636" z3="-0.965551"/>
    <atom id="a12" elementType="H" x3="-1.667705" y3="-0.920662" z3="-0.965616"/>
    <atom id="a13" elementType="O" x3="-0.990718" y3="-0.000059" z3="0.825260"/>
  </atomArray>
  <bondArray>
    <bond atomRefs2="a12 a10" order="1"/>
    <bond atomRefs2="a11 a10" order="1"/>
    <bond atomRefs2="a8 a6" order="1"/>
    <bond atomRefs2="a3 a2" order="1"/>
    <bond atomRefs2="a10 a1" order="1"/>
    <bond atomRefs2="a10 a13" order="1"/>
    <bond atomRefs2="a1 a2" order="1"/>
    <bond atomRefs2="a1 a6" order="1"/>
    <bond atomRefs2="a1 a13" order="1"/>
    <bond atomRefs2="a2 a4" order="1"/>
    <bond atomRefs2="a2 a5" order="1"/>
    <bond atomRefs2="a6 a7" order="1"/>
    <bond atomRefs2="a6 a9" order="1"/>
  </bondArray>
  <propertyList>
    <property title="program">
      <scalar>Gaussian 09, Revision D.01</scalar>
    </property>
    <property title="basis">
      <scalar>6-311++G(d,p) (5D, 7F)</scalar>
    </property>
    <property title="File Format">
      <scalar>g03</scalar>
    </property>
```

```
    <property title="Energy" dictRef="me:ZPE">
      <scalar units="kJ/mol">-74.51</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.9854</scalar>
    </property>
    <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
      <array units="cm-1">
        189.40 231.31 358.14 369.56 407.26 420.62 729.81 864.22 918.96 964.50
        969.77 1022.98 1094.62 1144.94 1162.31 1181.05 1303.79 1405.54 1422.64
        1438.09 1479.20 1493.93 1500.02 1516.33 1556.44 3055.32 3058.99 3116.68
        3127.26 3131.24 3148.40 3149.96 3208.99
      </array>
    </property>
    <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">0.219 0.186 0.131 </array>
    </property>
    <property title="Symmetry Number" dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:sigma" default="true">
      <scalar>5.0</scalar>
    </property>
    <property dictRef="me:epsilon" default="true">
      <scalar>70.0</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">72</scalar>
    </property>
  </propertyList>


  <me:DOSCMethod>ClassicalRotors</me:DOSCMethod>

</molecule>
<molecule id="OH" description="OH radical">
  <atomArray>
    <atom id="a1" elementType="O" />
    <atom id="a2" elementType="H" />
  </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">19.2438</array>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>0.9854</scalar>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3722.0</array>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:electronicExcitation">
      <array units="cm-1">139.7</array>
    </property>
  </propertyList>
  <me:DOSCMethod xsi:type="ClassicalRotors"/>
</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="N"/>
    <propertyList>
      <property dictRef="me:epsilon">
        <scalar>48.0</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>3.90</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">28.0</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>

  </molecule>

</moleculeList>

<reactionList>
  <reaction id="R1">
    <reactantList>
      <reactant>
        <molecule ref="QOOH" role="modelled"/>
      </reactant>
    </reactantList>
    <productList>
      <product>
        <molecule ref="DMO" role="sink"/>
      </product>
      <product>
        <molecule ref="OH" role="sink"/>
      </product>
    </productList>
    <me:transitionState>
      <molecule ref="TS" role="transitionState"/>
    </me:transitionState>
```

<me:MCRCMethod name="SimpleRRKM"/>
</reaction>
</reactionList>

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

<me:PTpair units="Torr" P="50" T="295" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="6169.730729">20073.01585</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="104.21" T="296" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="16195.98209">53942.39441</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="350.77" T="293" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="15915.59297">52903.38316</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="61.4806" T="283" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="6626.455817">22053.13636</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="107.34" T="283" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="10442.55781">34776.60972</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="40.756" T="283" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="6861.126687">22649.55677</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="202.55" T="282" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="13192.45303">43969.997</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="26.3963" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="2261.218535">6440.61</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="37.177" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="4398.308504">14383.04042</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="39.7613" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="3209.536865">9637.49095</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="24.1753" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="3328.975635">10994.94233</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="80.0903" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="7057.084926">23470.24499</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="162.75" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="9894.287673">32844.09362</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="336.5723" T="273" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="4511.589233">15031.46834</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="101.12" T="274" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="3285.617722">10892.49595</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="167.19" T="268" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="5273.268847">16820.97302</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="11.415" T="255" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1" error="915.0214995">3041.36572</me:experimentalRate></me:PTpair>

<me:PTpair units="Torr" P="185.87" T="255" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="2222.302919">7406.76342</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="50.031" T="255" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="1416.593333">4717.7298</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="34.076" T="255" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="1352.389576">4503.1761</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="69.158" T="255" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="1070.639896">3564.87543</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="36.358" T="251" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="1258.122809">4184.53912</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="38.1422" T="251" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="1766.83145">5865.21665</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="201.71" T="251" precision="d"><me:bathGas>He</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="2061.99702">6867.02119</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="10.354" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="9117.647217">30195</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="19.797" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="10440.83086">34577</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="30.41" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="13219.45612">43779</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="39.908" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="13778.07998">45629</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="59.922" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="16401.49839">54317</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="80.462" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="19455.81207">64432</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="98.396" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="16578.74823">54904</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="103.45" T="298" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="23954.75144">79331.18079</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="50.5679" T="277" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="3874.844273">12905.01093</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="109.33" T="275" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="4504.782712">15010.29477</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="22.5843" T="275" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="6523.474726">21697.37371</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="51.8153" T="275" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="11863.94567">39386.23472</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="8.6853" T="275" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="3380.836168">11247.66756</me:experimentalRate></me:PTpair>
<me:PTpair units="Torr" P="192.44" T="275" precision="d"><me:bathGas>N2</me:bathGas><me:experimentalRate ref1="QOOH" ref2="QOOH" refReaction="R1"
error="4875.078212">16161.52442</me:experimentalRate></me:PTpair>

<me:PTpair units="Torr" P="1" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="298" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="293" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="283" bathGas="He" precision="d" />

<me:PTpair units="Torr" P="10" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="283" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="273" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="268" bathGas="He" precision="d" />

<me:PTpair units="Torr" P="50" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="268" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="125" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="255" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="2" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="5" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="10" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="20" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="30" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="50" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="75" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="100" T="251" bathGas="He" precision="d" />

<me:PTpair units="Torr" P="125" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="150" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="200" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="225" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="250" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="275" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="300" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="325" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="350" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="375" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="400" T="251" bathGas="He" precision="d" />
<me:PTpair units="Torr" P="1" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="2" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="5" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="10" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="20" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="30" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="50" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="75" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="100" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="125" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="150" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="200" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="225" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="250" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="275" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="300" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="325" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="350" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="375" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="400" T="298" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="1" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="2" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="5" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="10" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="20" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="30" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="50" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="75" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="100" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="125" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="150" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="200" T="277" bathGas="N2" precision="d" />

```
<me:PTpair units="Torr" P="225" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="250" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="275" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="300" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="325" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="350" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="375" T="277" bathGas="N2" precision="d" />
<me:PTpair units="Torr" P="400" T="277" bathGas="N2" precision="d" />

    </me:PTs>

  </me:conditions>

  <me:modelParameters>
    <me:grainSize units="cm-1">35</me:grainSize>
    <me:energyAboveTheTopHill>30.</me:energyAboveTheTopHill>
  </me:modelParameters>

  <me:control>
    <me:calcMethod xsi:type="me:marquardt">
      <me:MarquardtIterations>40</me:MarquardtIterations>
      <me:MarquardtTolerance>0.0001</me:MarquardtTolerance>
      <me:MarquardtDerivDelta>1.e-03</me:MarquardtDerivDelta>
    </me:calcMethod>
    <me:testDOS />
    <me:eigenvalues>1</me:eigenvalues>
  </me:control>

</me:mesmer>
```