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

Supplemental Information for:

Reaction Kinetics of OH + HNO_3 under conditions relevant to the Upper Troposphere/Lower Stratosphere

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1 Calibration of the Photolysis Induced Fluorescence (PIF) detection method for HNO_3

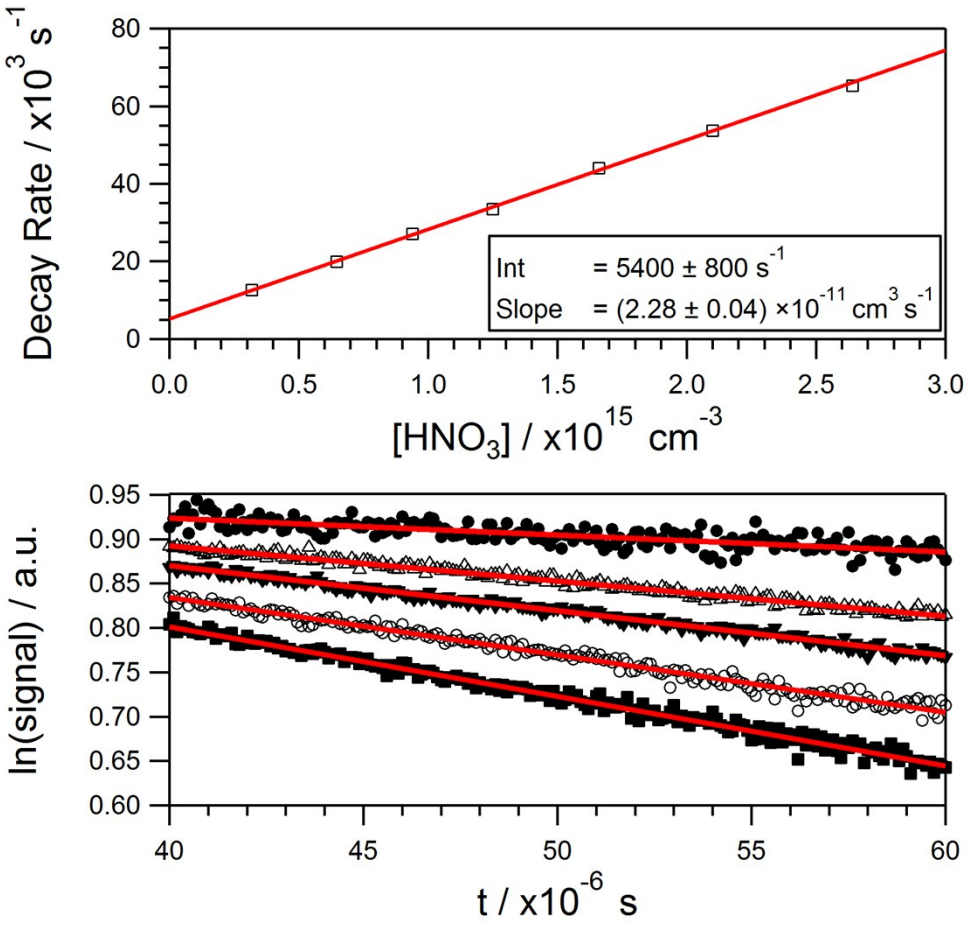

Figure S 1: Exponential decay fit (bottom panel) to determine the NO (A → X) fluorescence decay rate as a function of [HNO_3] (top panel) from the two-photon excitation of HNO_3 at 248 nm. Data collected at 200 Torr N_2, 298 K, 100 ns bin integration, 2000 laser shots at 20 Hz excimer repetition frequency.

2 Characterization of the *in-situ* VUV absorption axis

The *in-situ* detection of HNO_3 was complicated by the condensation of HNO_3 onto internal surfaces of the cell (copper shroud and Suprasil windows) at temperatures lower than ambient (HNO_3 freezing point ~230 K). Early attempts using the *in-situ* apparatus with windows on both ends of the insert arms led to inconsistent [HNO_3] measurements and erroneous $k_{OH+HNO3}$ determinations. To counter-act the uptake on HNO_3, the inside windows of the absorption axis inserts were removed, so that N_2 purge gas could be flowed through the inserts. The N_2 purge

flow was maintained at ~15% of the total flow and was directed through equal length tubing to maintain an even flow of gas through both inserts.

A set of characterization experiments were performed in a bulk flow of N_2 gas at 50 – 750 Torr and 298 – 235 K, using identical flows and parameters from the OH + HNO_3 kinetics experiments. Gas samples, N_2O and CF_3Br, were introduced pure, and liquid samples of CH_3OH, CH_3CH_2OH, $(CH_3)_2CO$, and HNO_3 (1:3 of HNO_3:H_2SO_4) were entrained into the gas phase using a bubbler with a flow of N_2 gas. Concentrations of gas phase samples were determined from their diluted flow into the bulk and liquid samples were determined using their respective Antoine coefficients [1, 2] and the bubbler temperature, pressure and flow rate.

Previously, compounds with well characterized cross-sections at 185 nm were introduced to the cell over a range of concentrations to determine the pathlength, l. However, when using the purged window apparatus, inconsistencies were observed in the measured effective pathlength, l_{eff}, as a result of mixing of the purge gas with the bulk flow. A comparison of several absorbers conducted at 500 Torr and 298 K revealed a dependence on the determined purged pathlength and the chosen absorber, which weakly correlated with the respective diffusion coefficients (assumed approximate correlation with inverse molecular mass), the values for which are displayed in Table S1.

Species	l_{eff} **/ cm**	**M / g mol^{-1}**
CF_3Br	16.8	150
$HONO_2$	11.9	63
$(CH_3)_2CO$	18.3	58
CH_3CH_2OH	8.6	46
N_2O	10.5	44
CH_3OH	12.0	32

Table S1: Effective pathlength, l_{eff}, determined using respective species, compared to the molecular mass.

As a result of the dependence of l_{eff} on the absorber used, it was important to characterize l_{eff} using HNO_3 as the absorber for the OH + HNO_3 kinetics experiments. Two methods were used: (1) comparison/evaluation using the *ex-situ* absorption cell and (2) measuring the difference in HNO_3 absorption between HNO_3/N_2 bulk with N_2 purge (normal operation) and flowing the HNO_3/N_2 mix through the purge inlets (non-purged). As the total pathlength of the non-purged absorption measurement is well defined, the effective pathlength when under normal operation can be determined with the comparison of the two absorption measurements. The effective pathlength measurements are listed in Table S2, showing good agreement between both methods. The pathlength was evaluated across the 50 – 750 Torr N_2 and 298 – 250 K temperature range, as used in the OH + HNO_3 study. No change in l_{eff} was observed with respect to cell temperature. Hence, the values for each pressure shown in Table S2 were used across the temperature range for the respective pressures.

Pressure / Torr	**l_{eff} / cm**	**Uncertainty / cm**
50	11.5	0.4
100	11.7	0.9
200	11.5	0.3
350	10.5	0.6
500	11.9	0.7
750	10.1	0.6

Table S2: Effective pathlength, l_{eff}, as a function of N_2 pressure (298 K), measured with HNO_3 absorption at 185 nm using method (2) described in the text.

To evaluate the possible effect of the purge flow on measured OH chemical kinetics, the rate coefficient for the reaction of OH + Ethane was determined under identical flow conditions to the OH + HNO_3 experiments. Ethane was chosen as a reactant due to a pressure independent and comparable rate coefficient to that of OH + HNO_3 at 298 K (k_{OH} = (2.5 ± 0.2) × 10^{-13} cm^3 s^{-1} [3]). Therefore, any changes in the rate coefficient due to introduction of the N_2 purge gas could be attributed to disruption of the reaction volume in the center of the reaction cell. No deviations in the rate coefficient for the reaction of OH + Ethane were observed under the flow

conditions used at 50 – 750 Torr or 298 – 250 K, suggesting that the reaction volume was not being perturbed by the purge gas flow.

3 Atmospheric modelling

STOCHEM is a global 3-dimensional chemistry transport model, in which the troposphere is divided into 50,000 air parcels which are advected every three hours using a 4th order Runge-Kutta scheme via a Lagrangian approach allowing the chemistry and transport processes to be uncoupled [4]. It is an offline model with the transport and radiation driven by archived meteorological data from the UK Meteorological office Unified Model which operates at a grid resolution of 1.25° longitudes by 0.83° latitude and twelve unevenly spaced vertical levels, with an upper boundary up to 100 hPa [5]. A detailed description of the meteorological parameterizations (e.g. vertical coordinate, advection scheme, boundary layer treatment, turbulence, inter-parcel exchange and convective mixing) in STOCHEM model can be found in Collins*, et al.* (1997), and Derwent*, et al.* (2008).

The chemical mechanism in the model is the common representative intermediate mechanism version 2 and reduction 5 (CRI v2-R5). A detailed description of CRI mechanism development has been presented in several literature publications [8-10]. This mechanism is directly traceable to the MCM v3.2 mechanism (http://mcm.leeds.ac.uk/CRI/), and it has been evaluated indirectly against measurement and chamber studies. In the current CRI chemistry scheme, each air parcel contains the concentration of 229 trace gases, which participate in 526 gas phase reactions and 96 photolysis reactions.

The model species are produced and lost by gas-phase reactions and photolysis. The rate coefficients of these reactions are specified as functions of temperature and incident light (values taken from either the MCM and/or the Jet Propulsion Laboratory kinetic evaluation

reports (http://jpldataeval.jpl.nasa.gov/), assuming perfect mixing within any given air parcel. The concentration of each chemical species is then updated using a backward Euler integration with a time step of five minutes [6].

The photolysis rate of a given species in STOCHEM-CRI is calculated using the following integral (equation I).

$$J_A = \int_0^\infty F(\lambda)\sigma_A(\lambda)\varphi_A(\lambda)d\lambda \qquad \text{(I)}$$

J_A represents the photolysis rate of compound A, $F(\lambda)$ represents the spherically integrated actinic flux at a given wavelength, $\sigma_A(\lambda)$ represents the cross section of compound A, at a given wavelength and $\varphi_A(\lambda)$ represents the quantum yield for dissociation of compound A, at a given wavelength. The cross section and quantum yields data are taken from the recommendations of either the JPL kinetic evaluation reports or the International Union of Pure and Applied Chemistry (IUPAC) data evaluations [11, 12]. Spherically integrated actinic fluxes are calculated over 106 wavelength intervals within the range 200 to 660 nm for a given air parcel using a variant of the one dimensional two stream model [13]. The photolysis rate is calculated explicitly for each air parcel at a time resolution of one hour, and then linearly interpolated with respect to time to achieve the 5-minute resolution values which are used in the chemical integration.

Surface, stratospheric and three-dimensional emissions are the emissions used in STOCHEM-CRI model. All emissions are converted into molecules per second per grid square, and are implemented as additional terms in the production flux for a given chemical species rather than five-minute step changes. The surface emissions totals for CO, NO_x, and non-methane volatile organic compounds (NMVOC) employed in the model were adapted from the Precursor of Ozone and their Effects in the Troposphere (POET) inventory [14] for the year 1998. Emissions total for CH_4 have been taken from an inverse model study [15], except for the oceanic emission,

which is taken from a tropospheric global model [16]. More details about the surface emissions data used in the model can be found in Khan*, et al.* (2014). Emissions from biomass Burning, vegetation, oceanic, and soil are distributed using monthly two-dimensional source maps at a 5° longitude by 5° latitude grid resolution [18]. Anthropogenic surface distributions for CH_4, CO, NO_X and VOC have been developed for the year 2000 by the International Institute for Applied Systems Analysis (IIASA) and are described in Cofala*, et al.* (2005).

The Lagrangian cells within the model are kept below 100 hPa by imposing a fixed lid to the model. In reality, there would be exchanges between the troposphere and the stratosphere. In order to represent this air exchange, stratospheric sources of ozone and HNO_3 are calculated as two-dimensional inputs in the top layer of the model, calculated using a three hourly vertical wind fields and monthly ozone fields [20]. The emissions are distributed on a resolution of 5° longitude by 5° latitude at a vertical coordinate of $\eta = 0.1$. Based on the work of Murphy and Fahey (1994), the HNO_3 flux is calculated as one thousandth of the ozone flux by mass of N.

The aircraft and lightning NO_x sources are distributed in a three-dimensional way within STOCHEM-CRI. Lightning is an important source of NO_x in the free troposphere, and the distribution in this model is parameterized based on a model simulated monthly two-dimensional fields of convective cloud top heights [22]. The emissions are distributed evenly by mass between the convective cloud top height and the surface. The lightning emissions are input on a resolution of 5° longitude by 5° latitude at a vertical resolution of $\Delta\eta = 0.1$. The emissions are scaled to give an annual emission of 5 Tg(N)/yr. The implementation of aircraft emission is the same as for lightning, using civil and military aircraft emission data taken from NASA inventories for 1992, which amounted to 0.85 Tg yr^{-1} of N globally [23].

When Lagrangian air parcels are within the boundary layers, the species within these air parcels can be lost through wet and dry deposition. The rate of dry deposition is dependent on the

deposition velocities for individual species, which varies on whether the air parcel is over land or ocean. The dry deposition velocities of the species are incorporated in the model to account for dry deposition loss and are calculated using equation (II).

$$F_A = c_A v_d / H \qquad \text{(II)}$$

Where F_A represents the dry deposition flux of a given species A, c_A represents the species concentration, v_d represents the dry deposition velocity of the species A and H represents the height above ground level.

Soluble species can be removed from the atmosphere by precipitation, commonly referred as wet deposition. The rate of wet deposition is dependent on the species convective and dynamic scavenging coefficients which are species specific. The coefficients along with both precipitation rates and scavenging profiles are used to determine loss rates of species in an air parcel via this process. Two simulations were conducted to assess the impact of the new evaluation of the reaction, OH + HNO_3 on OH and NO_x/HNO_3 in the UT-LS: the one with JPL 2015 evaluation report (referred to as base case) and the other one with the data reported in the paper. Each of the simulations was run with meteorology from 1998 for a period of 24 months with the initial 12 months being discarded as a spin-up year.

4 Derivation of alternative analytical function for k_1

Reaction and rate coefficient numbers used in this scheme have been kept in-line with those in the main text. Using the scheme:

$$OH + HNO_3 \leftrightarrow IM1^* \qquad (6)$$

$$IM1^* + M \leftrightarrow IM1 \qquad (7)$$

$$IM1^* \rightarrow H_2O + NO_3 \qquad (8)$$

IM1 $\rightarrow$ H_2O + NO_3 (9)

OH loss can be described as:

$$\frac{d[OH]}{dt} = k_{-6}[IM1^*] - k_6[OH] = 0 \quad \text{(S.I)}$$

First apply the steady state approximation to [IM1]:

$$\frac{d[IM1]}{dt} = k_7[M][IM1^*] - (k_{-7}[M] + k_9)[IM1] = 0 \quad \text{(S.II)}$$

$$[IM1] = \frac{k_7[M][IM1^*]}{(k_{-7}[M] + k_{9)}} \quad \text{(S.III)}$$

Next apply the steady state approximation to [IM1*] and substitute in [IM1]:

$$\frac{d[IM1^*]}{dt} = k_6[OH] - (k_{-6} + k_8 + k_7[M])[IM1^*] + k_{-7}[M][IM1] = 0 \quad \text{(S.IV)}$$

$$[IM1^*] = \frac{k_6(k_{-7}[M] + k_9)[OH]}{((k_{-6} + k_8 + k_7[M])(k_{-7}[M] + k_9) + k_{-7}[M]\,k_7[M])} \quad \text{(S.V)}$$

Substitute [IM1*] into (S.I):

$$d[OH] = \frac{-k_6((k_{-6} + k_8 + k_7[M])(k_{-7}[M] + k_9))[OH]}{((k_{-6} + k_8 + k_7[M])(k_{-7}[M] + k_9) + k_{-7}[M]\,k_7[M])} - \frac{k_6k_{-7}[M]k_7[M][OH]}{((k_{-6} + k_8 + k_7[M])(k_{-7}[M] + k_9) + \frac{k_{-6}k_6(k_{-7}[M] + k_9)[OH]}{((k_{-6} + k_8 + k_7[M])(k_{-7}[M] + k_9) + k_{-7}[M]\,k_7[M])} \quad \text{(S.VI)}$$

Assume $k_{-6} \gg k_8 + k_7[M]$ and $k_{-6}k_9 >> k_{-7}[M]k_7[M]$:

$$k_1 = \frac{k_6}{k_{-6}}k_8 + \frac{k_6}{k_{-6}(k_{-7}[M] + k_9)}k_7[M]k_9 \quad \text{(S.VII)}$$

5 Master Equation Modelling

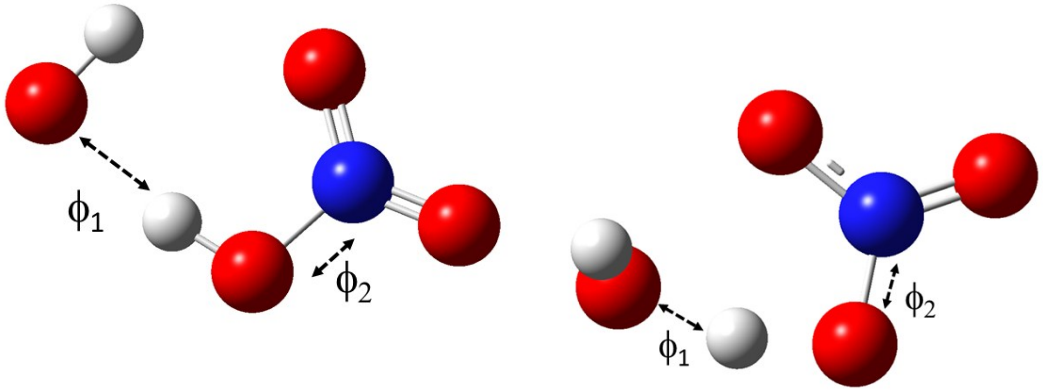

Figure S 2: Figure S2 Schematic showing bonds about which hindered rotation was considered in IM1 (left) and TS1 (right).

MESMER input file used in the current work

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  <atom id="a3" elementType="H" x3="1.045470" y3="0.780476" z3="-0.011278"/>
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            </me:HinderedRotorPotential>
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units="kJ/mol" UseSineTerms="yes">
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    </molecule>


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0.155292"/>
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            <atom id="a3" elementType="H" x3="2.225655" y3="0.141390" z3="2.600753"/>
            <atom id="a4" elementType="O" x3="-1.117018" y3="0.164806" z3="-0.758384"/>
            <atom id="a5" elementType="O" spinMultiplicity="2" x3="1.006833" y3="-
0.217265" z3="-0.559085"/>
            <atom id="a6" elementType="O" x3="1.917413" y3="-0.654272" z3="2.161839"/>
            <atom id="a7" elementType="H" x3="2.224225" y3="-0.583195" z3="1.253358"/>
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            <bond atomRefs2="a5 a1" order="1"/>
            <bond atomRefs2="a1 a2" order="2"/>
            <bond atomRefs2="a7 a6" order="1"/>
            <bond atomRefs2="a6 a3" 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="method">
                <scalar>M062x</scalar>
            </property>
            <property title="File Format">
                <scalar>g03</scalar>
            </property>
            <property title="Energy" dictRef="me:ZPE">
                <scalar units="kJ/mol" >-39.88 </scalar>
            </property>
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                <scalar>2.00 </scalar>
            </property>
            <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
                <array units="cm-1">68.00 112.67 144.09 210.15 241.58 443.28 505.12 689.85
818.49 948.30 1395.36 1641.25 1713.32 3869.55 3980.13 </array>
            </property>
            <property title="Rotational Constants" dictRef="me:rotConsts">
                <array units="cm-1">0.427 0.099 0.081 </array>
            </property>
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            <property title="Symmetry Number" dictRef="me:symmetryNumber">
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            </property>
         </propertyList>

         <me:DOSCMethod xsi:type="me:QMRotors"/>
      </molecule>

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            <atom id="a2" elementType="O" x3="0.048802" y3="0.005413" z3="1.374472"/>
            <atom id="a3" elementType="O" x3="-0.992840" y3="0.198812" z3="-0.457363"/>
            <atom id="a4" elementType="O" spinMultiplicity="2" x3="1.126663" y3="-
0.267343" z3="-0.426260"/>
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            <bond atomRefs2="a1 a2" order="2"/>
         </bondArray>
         <propertyList>
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            </property>
            <property title="basis">
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units="Hartree/Bohr2">0.88232541 -0.13033931 0.30500442 0.00522490 0.00299872
0.48549023 0.04548769 -0.02658627 0.00186381 0.03271638 -0.02651977 -0.07033030 -
0.00023496 -0.00264264 0.02208907 0.00213249 -0.00029162 -0.08782563 -0.00224252
0.00492774 0.26358909 -0.45886850 0.07361597 -0.19230755 -0.03815737 0.01317371 -
0.06056036 0.62424614 0.07251746 -0.11554788 0.03887134 0.01363422 0.02457382
0.01132371 -0.12239560 0.06263722 -0.24925893 0.05169540 -0.20507797 -0.03825504
0.00612693 -0.08934593 0.27279271 -0.05488471 0.24185072 -0.46894460 0.08330960
0.18521884 -0.04004670 0.01598870 0.06067038 -0.12722026 0.03624392 0.01472125
0.63621156 0.08434162 -0.11912623 -0.04163510 0.01559469 0.02366742 -0.01595983
0.03560592 0.02833685 -0.00293762 -0.13554222 0.06712197 0.24190154 -0.05440250 -
0.19258663 0.03863374 -0.01081971 -0.08641753 -0.01992480 0.00468966 0.05257318 -
0.26061048 0.06053255 0.22643099 </matrix>
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            <atom id="a3" elementType="H" x3="0.899492" y3="0.000000" z3="-0.296168"/>
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            <bond atomRefs2="a1 a2" order="1"/>
         </bondArray>
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            </property>
            <property title="basis">
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               <scalar units="kJ/mol" >0 </scalar>
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0.63018861 -0.04543198 0.00000000 -0.05313703 0.04687772 0.00000000 -0.00040712
0.00000000 0.00000000 0.00040285 0.00555596 0.00000000 -0.54417257 0.00372987
0.00000000 0.55982355 -0.50333793 0.00000000 0.16776517 -0.00144574 0.00000000 -
0.00928583 0.50478368 0.00000000 0.00028514 0.00000000 0.00000000 0.00000427
0.00000000 0.00000000 -0.00028942 0.10907219 0.00000000 -0.08601603 0.04940715
0.00000000 -0.01565098 -0.15847934 0.00000000 0.10166701 </matrix>
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  </moleculeList>
  <reactionList>

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        <molecule ref="OH" me:type="deficientReactant"/>
      </reactant>
      <reactant>
        <molecule ref="HNO3" me:type="excessReactant"/>
      </reactant>
      <product>
        <molecule ref="IM1" me:type="modelled"/>
      </product>
      <me:excessReactantConc>1E15</me:excessReactantConc>
      <me:MCRCMethod>MesmerILT</me:MCRCMethod>

      <me:preExponential >2.5E-11</me:preExponential>
      <me:activationEnergy>0.0</me:activationEnergy>
      <me:nInfinity >0.0</me:nInfinity>
      <me:TInfinity>293.0</me:TInfinity>
    </reaction>




    <reaction id="R_2">
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      </reactant>
      <product>
        <molecule ref="IM2" role="sink" />
      </product>
      <me:transitionState>
        <molecule ref="TS1" role="transitionState" />
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      <me:MCRCMethod name="SimpleRRKM"/>
      <me:tunneling>Eckart</me:tunneling>
```

```
        </reaction>

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              <molecule ref="TS2" role="transitionState" />
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calcVal="132.403">140.7171652</me:experimentalEigenvalue>
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error="&#x09;8.725269215&#x09;" calculated="20170912_160029"
calcVal="140.961">140.4523932</me:experimentalEigenvalue>
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default="true" bathGas="N2">
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calcVal="195.059">160.1684485</me:experimentalEigenvalue>
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default="true" bathGas="N2">
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calcVal="232.748">209.565157</me:experimentalEigenvalue>
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calcVal="259.286">202.24</me:experimentalEigenvalue>
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calcVal="163.467">205.6693836</me:experimentalEigenvalue>
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calcVal="194.362">223.2541982</me:experimentalEigenvalue>
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calcVal="267.812">274.481519</me:experimentalEigenvalue>
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default="true" bathGas="N2">
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calcVal="205.294">307.8691903</me:experimentalEigenvalue>
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<me:PTpair units="Torr" P="	350	" T="	223	" precision="d" default="true" bathGas="N2">
<me:bathGas>N2</me:bathGas>
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        <!--Stachnick-->

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        <me:experimentalEigenvalue EigenvalueID="1"  error="  10  ">  254
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        </me:PTpair>
        <me:PTpair  units="Torr"  P="  730  " T="  248  ">
        <me:bathGas>N2</me:bathGas>
        <me:experimentalEigenvalue EigenvalueID="1"  error="  20  ">  328
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        </me:PTpair>

        <me:PTpair  units="Torr"  P="  10  " T="  297  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="  10  ">  128
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        </me:PTpair>
        <me:PTpair  units="Torr"  P="  60  " T="  297  ">
        <me:bathGas>N2</me:bathGas>
        <me:experimentalEigenvalue EigenvalueID="1"  error="  15  ">  146
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        </me:PTpair>
        <me:PTpair  units="Torr"  P="  730  " T="  297  ">
<me:bathGas>N2</me:bathGas> <me:experimentalEigenvalue EigenvalueID="1"  error="
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        <!-- Brown He-->

        <me:PTpair  units="Torr"  P="  20  " T="  248  ">
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</me:experimentalEigenvalue>
        </me:PTpair>
        <me:PTpair  units="Torr"  P="  50  " T="  248  ">
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</me:experimentalEigenvalue>
        </me:PTpair>
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        <me:bathGas>He</me:bathGas>
        <me:experimentalEigenvalue EigenvalueID="1"  error="  23  ">  309
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        </me:PTpair>
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        <me:experimentalEigenvalue EigenvalueID="1"  error="  29  ">  310
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</me:experimentalEigenvalue>
        </me:PTpair>
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        <me:PTpair  units="Torr"  P="  20  " T="  296  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="8  ">  146
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        <me:experimentalEigenvalue EigenvalueID="1"  error="  10  ">  158
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        <me:PTpair  units="Torr"  P="  100  " T="  296  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="  9  ">  173
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  85
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        <me:PTpair  units="Torr"  P="  2  " T="  328  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  87
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        <me:PTpair  units="Torr"  P="  2  " T="  295  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  93
</me:experimentalEigenvalue>
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        <me:PTpair  units="Torr"  P="  2  " T="  278  ">
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  114
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  135
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        <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  150
</me:experimentalEigenvalue>
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</me:experimentalEigenvalue>
        </me:PTpair>

        <me:PTpair  units="Torr"  P="  2  " T="  358  ">
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          <me:experimentalEigenvalue EigenvalueID="1"  error="10  ">  85
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        <me:PTpair  units="Torr"  P="  2  " T="  328  ">
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</me:experimentalEigenvalue>
        </me:PTpair>

        <me:PTpair  units="Torr"  P="  1  " T="  278  ">
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</me:experimentalEigenvalue>
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</me:experimentalEigenvalue>
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  <me:bathGas>He</me:bathGas>
  <me:experimentalEigenvalue EigenvalueID="1"  error="2.6  ">  125.5
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair  units="Torr"  P="  1.55  " T="  253  ">
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  <me:experimentalEigenvalue EigenvalueID="1"  error="3">  108.5
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair  units="Torr"  P="  1.1  " T="  272  ">
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  <me:experimentalEigenvalue EigenvalueID="1"  error="5.2" >  93.8
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</me:PTpair>

<me:PTpair  units="Torr"  P="  1.1  " T="  301  ">
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  <me:experimentalEigenvalue EigenvalueID="1"  error="2.2" >  87.9
```

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<me:PTpair    units="Torr"    P="    10    " T="    301    ">
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   <me:experimentalEigenvalue EigenvalueID="1"     error="1.8" >    84
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair    units="Torr"    P="    2.8    " T="    324    ">
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   <me:experimentalEigenvalue EigenvalueID="1"     error="1" >    74.3
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</me:PTpair>

<me:PTpair    units="Torr"    P="    2.2    " T="    330    ">
   <me:bathGas>He</me:bathGas>
   <me:experimentalEigenvalue EigenvalueID="1"     error="3.4" >    75.2
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair    units="Torr"    P="    1.7    " T="    306    ">
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   <me:experimentalEigenvalue EigenvalueID="1"     error="1.6" >    88.2
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair    units="Torr"    P="    1.7    " T="    339    ">
   <me:bathGas>He</me:bathGas>
   <me:experimentalEigenvalue EigenvalueID="1"     error="1.8" >    83.7
</me:experimentalEigenvalue>
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   <me:bathGas>He</me:bathGas>
   <me:experimentalEigenvalue EigenvalueID="1"     error="6.4" >    75
</me:experimentalEigenvalue>
</me:PTpair>

<me:PTpair    units="Torr"    P="     20      " T="    208     ">
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      error="   29      ">      630     </me:experimentalEigenvalue>       </me:PTpair>
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error=" 12 "> 613 </me:experimentalEigenvalue> </me:PTpair>
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error=" 10 "> 646 </me:experimentalEigenvalue> </me:PTpair>
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error=" 4 "> 408 </me:experimentalEigenvalue> </me:PTpair>
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error=" 3 "> 396 </me:experimentalEigenvalue> </me:PTpair>
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error=" 10 "> 513 </me:experimentalEigenvalue> </me:PTpair>
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error=" 18 "> 584 </me:experimentalEigenvalue> </me:PTpair>
<me:PTpair units="Torr" P=" 17.7 " T=" 239 ">
<me:bathGas>N2</me:bathGas> <me:experimentalEigenvalue EigenvalueID="1"
error=" 3 "> 309 </me:experimentalEigenvalue> </me:PTpair>
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error=" 7 "> 309 </me:experimentalEigenvalue> </me:PTpair>
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error=" 3 "> 354 </me:experimentalEigenvalue> </me:PTpair>
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error=" 6 "> 354 </me:experimentalEigenvalue> </me:PTpair>
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error="5"> 340 </me:experimentalEigenvalue> </me:PTpair>
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error="2"> 214 </me:experimentalEigenvalue> </me:PTpair>
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error="3"> 254 </me:experimentalEigenvalue> </me:PTpair>
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error="3"> 254 </me:experimentalEigenvalue> </me:PTpair>
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<me:bathGas>N2</me:bathGas> <me:experimentalEigenvalue EigenvalueID="1"
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<me:PTpair   units="Torr"   P="    17.9   " T="   276    ">
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      error="  2      ">      159    </me:experimentalEigenvalue>      </me:PTpair>
<me:PTpair   units="Torr"   P="    18.2   " T="   276    ">
<me:bathGas>N2</me:bathGas> <me:experimentalEigenvalue EigenvalueID="1"
      error="  3      ">      169    </me:experimentalEigenvalue>      </me:PTpair>
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      error="  2      ">      167    </me:experimentalEigenvalue>      </me:PTpair>
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      error="  2      ">      160    </me:experimentalEigenvalue>      </me:PTpair>
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      error="  1      ">      162    </me:experimentalEigenvalue>      </me:PTpair>
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