Supplementary Information:

Experimental and Computational Studies of Criegee Intermediate Reactions with NH_3 and CH_3NH_2

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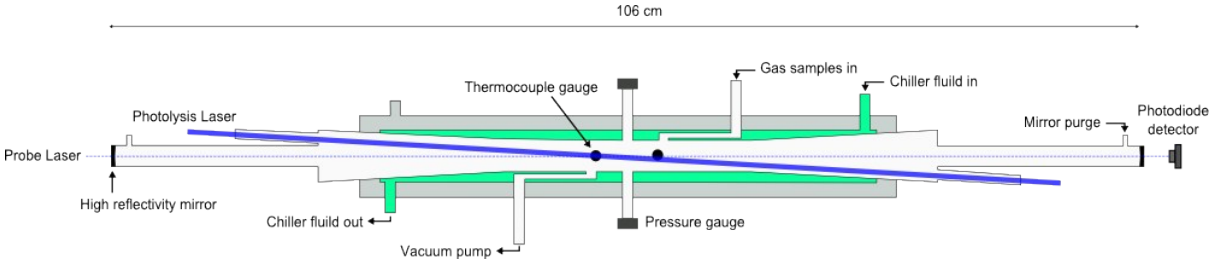

Figure S1: Schematic diagram of the variable temperature flow reactor used for measuring reaction of Criegee intermediates with NH_3 and CH_3NH_2. The bright green layer shows the jacket containing chiller fluid. The outer grey layer is a jacket containing air to insulate the reactor and chiller fluid from ambient temperature. The paths of the photolysis and probe CRDS lasers are shown by solid and dashed lines respectively.

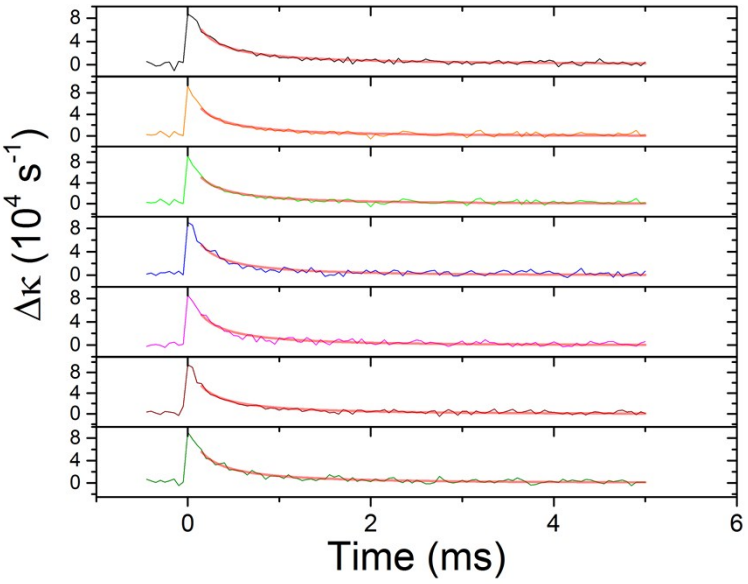

Figure S2: Bimolecular reaction of $(CH_3)_2COO$ with NH_3. The plot shows $(CH_3)_2COO$ decay traces obtained in the presence of various concentrations of NH_3, shown in Figure S3, at 10 Torr total pressure and 293 K. All the traces were corrected for depletion signal of the $(CH_3)_2CI_2$ precursor. The red traces show fits to equation E1 in the main text. The traces are shown separately for clarity.

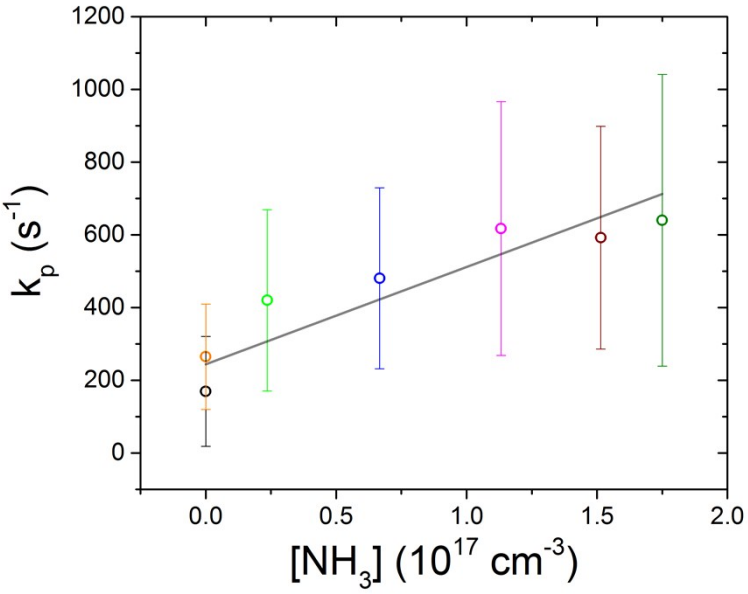

Figure S3: Bimolecular fit for the $(CH_3)_2COO$ + NH_3 reaction. The k_p values were obtained from the fits shown in Figure S2. The gradient of the linear fit gives the second-order rate coefficient for the reaction.

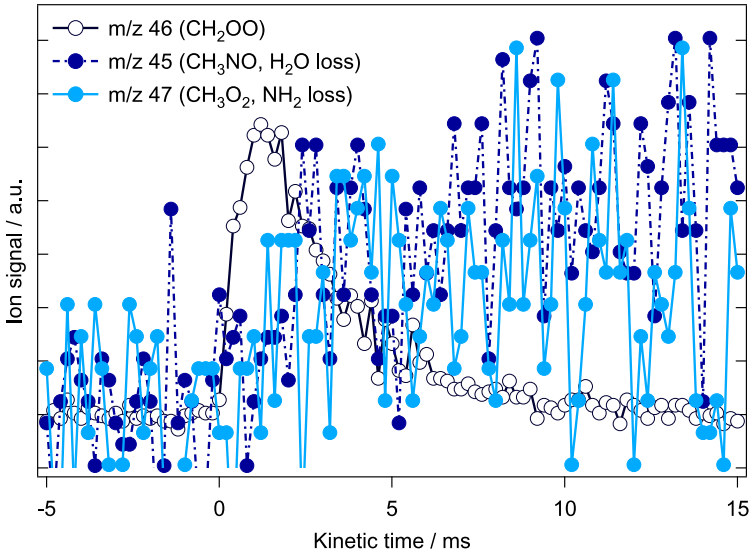

Figure S4: Kinetic profiles of the CH_2OO Criegee Intermediate (black open circles) in the presence of NH_3, and proposed daughter ion species from the ionization of predicted functionalized hydroperoxide products. Kinetic profiles were obtained from data recorded at a fixed photoionization energy of 10.5 eV.

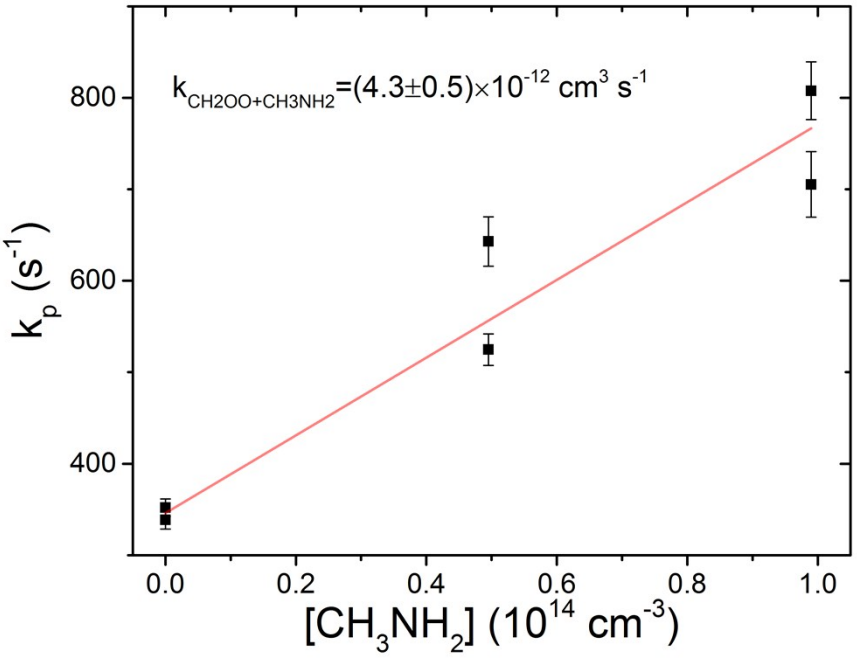

Figure S5: Bimolecular plot obtained from single exponential fits to Criegee Intermediate decays measured at a photoionization energy of 10.5 eV in the presence and absence of CH_3NH_2, yielding a bimolecular rate coefficient of (4.3 ± 0.5) × 10^{-12} cm^3 s^{-1} (1σ error from the weighted linear fit).

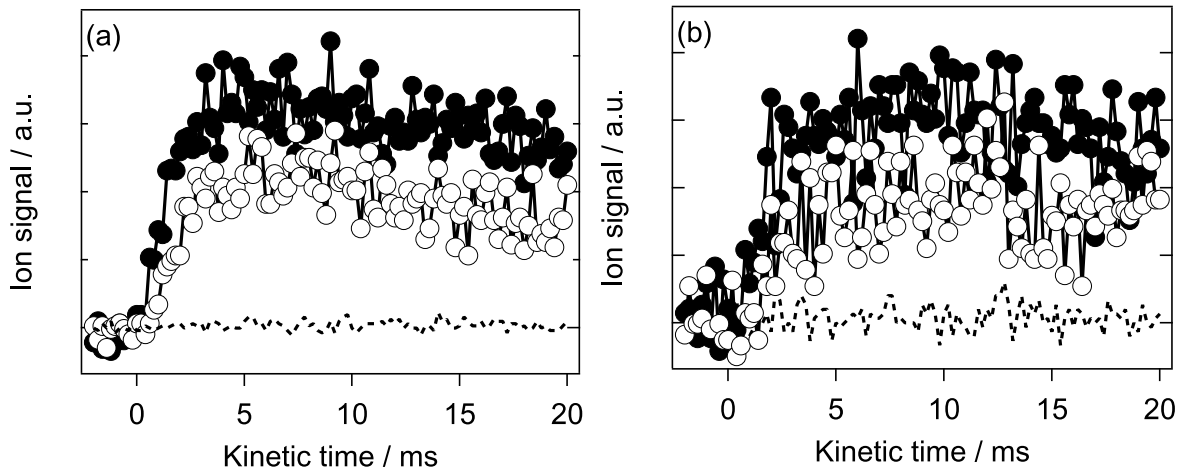

Figure S6: Temporal profiles of (a) m/z 44, and (b) m/z 59 species, from MPIMS measurements for the reaction of CH_2OO with CH_3NH_2. In the plots, [CH_3NH_2] = 0 (black dashed line), 4.95 × 10^{13} molecule cm^{-3} (black open circles) and 9.90 × 10^{13} molecule cm^{-3} (black closed circles).

Table S1: Rate coefficients k(p,T) for the $CH_2OO + NH_3$ reaction at various pressures and temperatures. The rate coefficient error shown are 2σ values obtained from the weighted linear fit. The temperature error shown is the difference between the inlet and outlet temperature values as shown in Figure S1.

Pressure (Torr)	Temperature (K)	k (10^{-13} cm^3s^{-1})
10	247.6±1.8	11.5±0.7
10	253.9±1.4	10.7±1.1
10	258.1±1.3	10.0±0.4
10	260.6±1.1	10.1±0.9
10	267.0±0.9	10.6±0.9
10	276.0±0.6	8.2±0.8
10	284.5±0.3	8.0±0.6
10	289.5±0.1	7.9±0.4
10	293.2±0.0	8.4±0.9
10	294.4±0.0	9.2±0.4
10	293.8±0.1	7.7±0.6
10	294.5±0.0	8.4±0.3
10	302.1±0.2	8.1±0.5
10	302.1±0.2	7.8±0.2
10	302.2±0.2	8.1±0.7
10	311.3±0.4	8.4±0.8
10	311.4±0.4	7.1±0.6
10	320.4±0.6	7.5±0.2
10	320.2±0.5	6.8±0.6
20	293	8.7±0.3
45	293	7.8±2.0
52	293	8.6±0.8
60	293	7.5±0.7
70	293	8.6±0.8
90	293	9.1±1.0

Table S2: Rate coefficients k(p,T) for the CH_2OO + CH_3NH_2 reaction at various pressures and temperatures. The rate coefficient error shown are 2σ values obtained from the weighted linear fit. The temperature error shown is the difference between the inlet and outlet temperature values as shown in Figure S1.

Pressure (Torr)	Temperature (K)	k (10^{-12} cm^3s^{-1})
10	263.0±1.0	6.64±0.66
10	267.4±0.8	6.61±0.60
10	275.8±0.5	6.35±1.01
10	288.5±0.2	5.52±0.34
10	297.5±0.1	4.41±0.70
10	311.2±0.4	3.60±0.64
50	258.2±1.0	7.40±0.80
50	266.8±0.8	5.96±0.61
50	275.6±0.5	5.13±1.71
50	284.4±0.2	5.34±1.28
50	293.6±0.0	4.74±0.29
50	302.2±0.2	4.75±0.30
50	311.3±0.4	2.80±1.32
10	293	5.73±0.52
20	293	5.69±0.28
30	293	5.85±0.69
60	293	5.38±0.47
100	293	5.38±0.33

Table S3: Stationary point energies for key structures involved in the $CH_2OO + NH_3$ reaction computed at various levels of theory. All the energies and frequencies are computed for CCSD(T)(F12)/cc-pVDZ-F12 optimised structures. Values are quoted in kJ mol^{-1} relative to the reactants.*

	HF+CABS			dCCSD(F12*)(T)			ZPVE			B3LYP	CCSD(T)	Best
	DZ	TZ	QZ	DZ	TZ	QZ	DZ	TZ	QZ			
Complex	-32.3	-32.2	-32.1	2.4	2.4	2.4	2.1	2.3	2.4	6.7	7.7	-19.6
TS	-21.3	-21.0	-20.9	1.9	2.0	2.1	2.7	3.0	3.2	11.2	12.8	-2.7
Products	-222.9	-222.7	-222.6	0.3	0.9	1.3	12.9	14.0	14.5	20.6	22.2	-184.6

Table S4: Stationary point energies for key structures involved in the $CH_2OO + CH_3NH_2$ reaction computed at various levels of theory. All the energies and frequencies are computed at CCSD(T)(F12)/cc-pVDZ-F12 optimised structures. Values are quoted in kJ mol^{-1} relative to the reactants.*

	HF+CABS		dCCSD(F12*)(T)		ZPVE		B3LYP	CCSD(T)	Best
	DZ	TZ	DZ	TZ	DZ	TZ			
Complex	-32.3	-32.1	-0.4	-0.6	1.6	1.7	6.8	6.6	-24.4
TS	-31.0	-30.7	-0.6	-0.7	1.8	1.9	8.4	8.8	-20.7
Products	-229.8	-229.5	-7.1	-6.5	11.4	12.3	17.1	17.8	-205.9

Table S5: Comparison between theoretical rate coefficients from the full master equation treatment k_{ME} and a steady state treatment k_{CAN} based on canonical rate coefficients from MESMER for the CH_2OO + NH_3 reaction. Also included are the individual rate coefficients k_4, k_{-4} and k_5. k_4 is formulated here as a pseudo first order rate coefficient with the master equation excess reactant concentration of 1×10^{15} molecule cm^{-3}.

Temperature (K)	k_{ME} (10^{-13} cm^3s^{-1})	k_{CAN} (10^{-14} cm^3s^{-1})	k_4 (10^{-10} cm^3 s^{-1})	k_{-4} (10^{11} s^{-1})	k_5 (10^8 s^{-1})
247.6	10.3	11.6	1.01	1.09	1.26
253.9	9.97	11.1	1.01	1.38	1.52
258.1	9.76	10.8	1.01	1.59	1.71
260.6	9.63	10.6	1.01	1.73	1.83
267.0	9.36	10.2	1.01	2.13	2.17
276.0	9.00	9.74	1.00	2.80	2.72
284.5	8.70	9.33	1.00	3.56	3.31
289.5	8.53	9.11	1.00	4.07	3.69
293.2	8.41	8.96	1.00	4.48	4.00
293.8	8.40	8.94	1.00	4.55	4.05
294.4	8.38	8.91	1.00	4.62	4.10
294.5	8.38	8.91	1.00	4.63	4.11
302.1	8.18	8.63	1.00	5.58	4.79
302.1	8.18	8.63	1.00	5.58	4.79
302.2	8.17	8.63	1.00	5.59	4.80
311.3	7.94	8.33	1.00	6.88	5.71
311.4	7.93	8.33	1.00	6.90	5.72
320.4	7.74	8.08	1.00	8.36	6.73

Table S6: Comparison between theoretical rate coefficients from the full master equation treatment k_{ME} and a steady state treatment k_{CAN} based on canonical rate coefficients from MESMER for the CH_2OO + CH_3NH_2 reaction. Also included are the individual rate coefficients k_4, k_{-4} and k_5. k_4 is formulated here as a pseudo first order rate coefficient with the master equation excess reactant concentration of 1×10^{15} molecule cm^{-3}.

Temperature (K)	k_{ME} (10^{-12} cm^3s^{-1})	k_{CAN} (10^{-10} cm^3s^{-1})	k_4 (10^{-10} cm^3 s^{-1})	k_{-4} (10^{11} s^{-1})	k_5 (10^{11} s^{-1})
258.2	6.85	14.9	1.01	2.04	3.03
263.0	6.58	12.5	1.01	2.47	3.06
266.8	6.37	10.9	1.01	2.86	3.09
267.4	6.34	10.7	1.01	2.92	3.09
275.6	5.93	8.06	1.01	3.93	3.15
275.8	5.91	8.01	1.01	3.96	3.15
284.4	5.51	6.10	1.01	5.29	3.21
288.5	5.33	5.39	1.01	6.03	3.23
293.6	5.12	4.64	1.01	7.06	3.26
297.5	4.97	4.16	1.01	7.94	3.28
302.2	4.79	3.66	1.01	9.09	3.31
311.2	4.47	2.90	1.01	11.6	3.36
311.3	4.46	2.89	1.01	11.7	3.36

Example MESMER input for NH_3 + CH_2OO reaction

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<property title="Vibrational Frequencies" dictRef="me:vibFreqs">
<array units="cm-1">202.96 236.24 388.16 488.72 613.08 788.44 877.18 972.42 1049.49
1103.50 1273.75 1350.79 1426.39 1432.20 1504.44 1665.62 3046.70 3104.87 3552.90 3646.77
3697.16 </array>
</property>
<property dictRef="me:epsilon">
<scalar>216.11</scalar>
</property>
```

```
      <property dictRef="me:sigma">
        <scalar>4.6</scalar>
      </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
      <me:deltaEDown units="cm-1">200.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod xsi:type="QMRotors"/>
  </molecule>
  </moleculeList>
<reactionList>
  <reaction id="R_1">
    <reactant>
      <molecule ref="NH3"  role="excessReactant" />
    </reactant>
    <reactant>
      <molecule ref="Criegee"  role="deficientReactant" />
    </reactant>
    <product>
      <molecule ref="complex"  role="modelled" />
    </product>
    <me:MCRCMethod xsi:type="MesmerILT">
      <me:preExponential>1.00e-10</me:preExponential>
      <me:activationEnergy  units="cm-1" >0</me:activationEnergy>
      <me:nInfinity>0.0</me:nInfinity>
    </me:MCRCMethod>
  <me:excessReactantConc>1.0E15</me:excessReactantConc>
  </reaction>
  <reaction id="R_2">
    <reactant>
      <molecule ref="complex" role="modelled" />
    </reactant>
```

```
    <product>
     <molecule ref="Prod" role="sink" />
    </product>
    <me:transitionState>
     <molecule ref="ts" role="transitionState" />
    </me:transitionState>
    <me:MCRCMethod name="SimpleRRKM"/>
    <me:tunneling>Eckart</me:tunneling>
   </reaction>


  </reactionList>
 <me:conditions>
   <me:bathGas>N2</me:bathGas>
   <me:PTs>
     <!-- <me:PTpair units="Torr" P="10" T="294.5"><me:experimentalEigenvalue EigenvalueID="1"
error="10">91</me:experimentalEigenvalue></me:PTpair>
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error="8">86</me:experimentalEigenvalue></me:PTpair>
      <me:PTpair units="Torr" P="60" T="294.5"><me:experimentalEigenvalue EigenvalueID="1"
error="7">75</me:experimentalEigenvalue></me:PTpair>
      <me:PTpair units="Torr" P="52" T="294.5"><me:experimentalEigenvalue EigenvalueID="1"
error="8">86</me:experimentalEigenvalue></me:PTpair>
      <me:PTpair units="Torr" P="45" T="294.5"><me:experimentalEigenvalue EigenvalueID="1"
error="20">78</me:experimentalEigenvalue></me:PTpair>
      <me:PTpair units="Torr" P="20" T="294.5"><me:experimentalEigenvalue EigenvalueID="1"
error="3">87</me:experimentalEigenvalue></me:PTpair>-->
    <me:PTpair units="Torr" P="10" T="247.6"><me:experimentalEigenvalue EigenvalueID="1"
error="7.09">115</me:experimentalEigenvalue></me:PTpair>
    <!--<me:PTpair units="Torr" P="10" T="253.9"><me:experimentalEigenvalue EigenvalueID="1"
error="11.3">107</me:experimentalEigenvalue></me:PTpair>
    <me:PTpair units="Torr" P="10" T="258.1"><me:experimentalEigenvalue EigenvalueID="1"
error="4.1">100</me:experimentalEigenvalue></me:PTpair>
    <me:PTpair units="Torr" P="10" T="260.6"><me:experimentalEigenvalue EigenvalueID="1"
error="8.6">101</me:experimentalEigenvalue></me:PTpair>
  <me:PTpair units="Torr" P="10" T="267.0"><me:experimentalEigenvalue EigenvalueID="1"
error="9.0">106</me:experimentalEigenvalue></me:PTpair>
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<me:PTpair units="Torr" P="10" T="276"><me:experimentalEigenvalue EigenvalueID="1" error="7.61">81.6</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="284.5"><me:experimentalEigenvalue EigenvalueID="1" error="6.22">79.9</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="289.5"><me:experimentalEigenvalue EigenvalueID="1" error="3.52">79.3</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="293.2"><me:experimentalEigenvalue EigenvalueID="1" error="8.9">83.6</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="294.4"><me:experimentalEigenvalue EigenvalueID="1" error="4.06">92.4</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="293.8"><me:experimentalEigenvalue EigenvalueID="1" error="5.78">77.4</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="294.5"><me:experimentalEigenvalue EigenvalueID="1" error="2.69">84.1</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="302.1"><me:experimentalEigenvalue EigenvalueID="1" error="4.87">80.7</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="302.1"><me:experimentalEigenvalue EigenvalueID="1" error="1.49">78.3</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="302.2"><me:experimentalEigenvalue EigenvalueID="1" error="7.89">80.7</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="311.3"><me:experimentalEigenvalue EigenvalueID="1" error="7.89">83.7</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="311.4"><me:experimentalEigenvalue EigenvalueID="1" error="5.58">71.3</me:experimentalEigenvalue></me:PTpair>

<me:PTpair units="Torr" P="10" T="320.4"><me:experimentalEigenvalue EigenvalueID="1" error="9.0">75.0</me:experimentalEigenvalue></me:PTpair>-->

<me:PTpair units="Torr" P="10" T="320.2"><me:experimentalEigenvalue EigenvalueID="1" error="6.38">68.4</me:experimentalEigenvalue></me:PTpair>

</me:PTs>

</me:conditions>

<me:modelParameters>

<me:grainSize units="cm-1">10</me:grainSize>

<me:energyAboveTheTopHill>30.</me:energyAboveTheTopHill>

</me:modelParameters>

<me:control>

<!--<me:calcMethod xsi:type="me:marquardt">

<me:MarquardtIterations>10</me:MarquardtIterations>

```
    <me:MarquardtTolerance>0.1</me:MarquardtTolerance>
    <me:MarquardtDerivDelta>1.e-02</me:MarquardtDerivDelta>
  </me:calcMethod>-->
  <me:printSpeciesProfile/>
<me:testRateConstants/>
  <me:printGrainedSpeciesProfile/>
  <me:eigenvalues>3</me:eigenvalues>
 </me:control>
</me:mesmer>
```

Example MESMER input for $CH_2OO + CH_3NH_2$

```
<?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>NH2CH3 + Criegee</me:title>
   <moleculeList>
      <molecule id="NH2CH3" xmlns="http://www.xml-cml.org/schema">
         <atomArray>
            <atom id="a1" elementType="N" x3="0.000000" y3="-0.071919" z3="-0.721253"/>
            <atom id="a2" elementType="C" x3="0.000000" y3="0.013616" z3="0.740309"/>
            <atom id="a3" elementType="H" x3="0.000000" y3="1.033003" z3="1.141405"/>
            <atom id="a4" elementType="H" x3="-0.809210" y3="0.404508" z3="-1.097147"/>
            <atom id="a5" elementType="H" x3="0.809210" y3="0.404508" z3="-1.097147"/>
            <atom id="a6" elementType="H" x3="0.878164" y3="-0.502428" z3="1.126941"/>
            <atom id="a7" elementType="H" x3="-0.878164" y3="-0.502428" z3="1.126941"/>
         </atomArray>
         <bondArray>
            <bond atomRefs2="a4 a1" order="1"/>
            <bond atomRefs2="a5 a1" order="1"/>
            <bond atomRefs2="a1 a2" order="1"/>
            <bond atomRefs2="a2 a6" order="1"/>
            <bond atomRefs2="a2 a7" order="1"/>
            <bond atomRefs2="a2 a3" order="1"/>
         </bondArray>
         <propertyList>
            <property title="Energy" dictRef="me:ZPE">
               <scalar units="kJ/mol" >0 </scalar>
            </property>
```

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">299.68 855.21 978.12 1072.12 1184.05 1360.35 1467.84 1514.18 1532.85 1672.06 3006.00 3088.21 3125.41 3516.44 3598.61 </array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>3 </scalar>

</property>

</propertyList>

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

</molecule>

<molecule id="Criegee" spinMultiplicity="3" xmlns="http://www.xml-cml.org/schema">

<atomArray>

<atom id="a1" elementType="C" spinMultiplicity="2" x3="0.000000" y3="0.244135" z3="-1.127237"/>

<atom id="a2" elementType="O" x3="0.000000" y3="-0.446241" z3="-0.066751"/>

<atom id="a3" elementType="O" spinMultiplicity="2" x3="0.000000" y3="0.200216" z3="1.107455"/>

<atom id="a4" elementType="H" x3="0.000000" y3="-0.327047" z3="-2.042958"/>

<atom id="a5" elementType="H" x3="0.000000" y3="1.323082" z3="-1.043933"/>

</atomArray>

<bondArray>

<bond atomRefs2="a4 a1" order="1"/>

<bond atomRefs2="a1 a5" order="1"/>

<bond atomRefs2="a1 a2" order="1"/>

<bond atomRefs2="a2 a3" order="1"/>

</bondArray>

<propertyList>

<property title="File Format">

<scalar>mpo</scalar>

</property>

<property title="Energy" dictRef="me:ZPE">

<scalar units="kJ/mol" >0 </scalar>

</property>

<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">

```
            <scalar>1.00 </scalar>
          </property>
          <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
            <array units="cm-1">537.23 657.15 893.88 934.34 1246.76 1340.72 1504.35 3144.13
3305.63 </array>
          </property>
          <property title="Symmetry Number" dictRef="me:symmetryNumber">
            <scalar>1 </scalar>
          </property>
        </propertyList>
        <me:DOSCMethod xsi:type="QMRotors"/>
      </molecule>
      <molecule id="complex" spinMultiplicity="3" xmlns="http://www.xml-cml.org/schema">
        <atomArray>
          <atom id="a1" elementType="C" spinMultiplicity="2" x3="0.149150" y3="-1.146497" z3="-
1.005727"/>
          <atom id="a2" elementType="O" x3="-0.512399" y3="-0.105892" z3="-1.227519"/>
          <atom id="a3" elementType="O" spinMultiplicity="2" x3="0.209596" y3="1.062706" z3="-
1.312140"/>
          <atom id="a4" elementType="N" x3="0.689074" y3="-0.094722" z3="1.405583"/>
          <atom id="a5" elementType="H" x3="1.227292" y3="-1.094129" z3="-0.978777"/>
          <atom id="a6" elementType="H" x3="-0.433318" y3="-2.050174" z3="-0.890964"/>
          <atom id="a7" elementType="H" x3="0.865898" y3="0.667027" z3="0.755116"/>
          <atom id="a8" elementType="H" x3="1.454542" y3="-0.110317" z3="2.066177"/>
          <atom id="a9" elementType="C" x3="-0.578106" y3="0.149459" z3="2.098288"/>
          <atom id="a10" elementType="H" x3="-0.783538" y3="-0.672071" z3="2.784485"/>
          <atom id="a11" elementType="H" x3="-0.606730" y3="1.086227" z3="2.662858"/>
          <atom id="a12" elementType="H" x3="-1.381652" y3="0.182951" z3="1.362163"/>
        </atomArray>
        <bondArray>
          <bond atomRefs2="a3 a2" order="1"/>
          <bond atomRefs2="a2 a1" order="1"/>
          <bond atomRefs2="a1 a5" order="1"/>
          <bond atomRefs2="a1 a6" order="1"/>
```

```
      <bond atomRefs2="a7 a4" order="1"/>
      <bond atomRefs2="a12 a9" order="1"/>
      <bond atomRefs2="a4 a8" order="1"/>
      <bond atomRefs2="a4 a9" order="1"/>
      <bond atomRefs2="a9 a11" order="1"/>
      <bond atomRefs2="a9 a10" order="1"/>
    </bondArray>
    <propertyList>
      <property title="Energy" dictRef="me:ZPE">
        <scalar units="kJ/mol" >-24.4 </scalar>
      </property>
      <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
        <scalar>1 </scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">62.51 73.02 112.67 145.51 170.33 259.24 435.26 518.95 675.92
842.27 922.84 981.86 1006.80 1072.15 1193.07 1237.60 1372.72 1396.67 1466.08 1511.60 1534.17
1546.37 1670.77 3018.45 3087.30 3120.96 3153.19 3306.21 3461.44 3578.81 </array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>3 </scalar>
      </property>
      <property dictRef="me:epsilon">
        <scalar>216.11</scalar>
      </property>
      <property dictRef="me:sigma">
        <scalar>4.6</scalar>
      </property>
    </propertyList>
    <me:energyTransferModel xsi:type="me:ExponentialDown">
      <me:deltaEDown units="cm-1">200.0</me:deltaEDown>
    </me:energyTransferModel>
    <me:DOSCMethod xsi:type="QMRotors"/>
```

```
    </molecule>
    <molecule id="ts">
      <atomArray>
        <atom id="a1" elementType="C" spinMultiplicity="2" x3="0.175668" y3="-1.127368" z3="-0.724912"/>
        <atom id="a2" elementType="N" x3="0.676143" y3="-0.008928" z3="1.251126"/>
        <atom id="a3" elementType="H" x3="0.799159" y3="0.742915" z3="0.571608"/>
        <atom id="a4" elementType="O" spinMultiplicity="2" x3="0.187169" y3="0.976665" z3="-1.436450"/>
        <atom id="a5" elementType="O" x3="-0.547285" y3="-0.190499" z3="-1.136676"/>
        <atom id="a6" elementType="H" x3="1.242831" y3="-1.081158" z3="-0.883594"/>
        <atom id="a7" elementType="H" x3="-0.346623" y3="-2.017418" z3="-0.397454"/>
        <atom id="a8" elementType="H" x3="1.498671" y3="-0.055064" z3="1.836637"/>
        <atom id="a9" elementType="C" x3="-0.535157" y3="0.223997" z3="2.037087"/>
        <atom id="a10" elementType="H" x3="-0.671478" y3="-0.586493" z3="2.752419"/>
        <atom id="a11" elementType="H" x3="-1.391022" y3="0.234812" z3="1.361508"/>
        <atom id="a12" elementType="H" x3="-0.527391" y3="1.172290" z3="2.580586"/>
      </atomArray>
      <bondArray>
        <bond atomRefs2="a4 a5" order="1"/>
        <bond atomRefs2="a5 a1" order="1"/>
        <bond atomRefs2="a6 a1" order="1"/>
        <bond atomRefs2="a1 a7" order="1"/>
        <bond atomRefs2="a3 a2" order="1"/>
        <bond atomRefs2="a2 a8" order="1"/>
        <bond atomRefs2="a2 a9" order="1"/>
        <bond atomRefs2="a11 a9" order="1"/>
        <bond atomRefs2="a9 a12" order="1"/>
        <bond atomRefs2="a9 a10" order="1"/>
      </bondArray>
      <propertyList>
        <property title="Energy" dictRef="me:ZPE">
          <scalar units="kJ/mol" upper="-16" lower="-24" stepsize="0.1">-22.4</scalar>
```

```
        </property>
        <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
          <scalar>1</scalar>
        </property>
        <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
          <array units="cm-1">84.58 137.59 160.34 207.13 383.09 505.75 547.00 751.77 810.20
945.15 1029.10 1047.81 1081.63 1194.73 1226.66 1369.63 1407.11 1466.77 1511.56 1534.72
1567.86 1671.30 3028.48 3095.00 3126.14 3146.19 3289.59 3402.66 3582.76 </array>
        </property>
        <property title="Symmetry Number" dictRef="me:symmetryNumber">
          <scalar> 3 </scalar>
        </property>
        <property title="ImaginaryFrequency" dictRef="me:imFreqs">
          <scalar units="cm-1">151.41 </scalar>
        </property>
      </propertyList>
      <me:DOSCMethod xsi:type="QMRotors"/>
    </molecule>
    <molecule id="Prod" xmlns="http://www.xml-cml.org/schema">
      <atomArray>
        <atom id="a1" elementType="C" x3="0.326883" y3="-0.857870" z3="-0.016248"/>
        <atom id="a2" elementType="N" x3="0.580908" y3="0.194868" z3="0.936006"/>
        <atom id="a3" elementType="O" x3="-0.569028" y3="-0.405500" z3="-1.008532"/>
        <atom id="a4" elementType="O" x3="0.110717" y3="0.660588" z3="-1.709198"/>
        <atom id="a5" elementType="H" x3="1.269445" y3="-1.165155" z3="-0.473908"/>
        <atom id="a6" elementType="H" x3="-0.193976" y3="-1.723571" z3="0.411080"/>
        <atom id="a7" elementType="H" x3="0.303897" y3="1.251480" z3="-0.962448"/>
        <atom id="a8" elementType="C" x3="-0.451883" y3="0.326366" z3="1.959579"/>
        <atom id="a9" elementType="H" x3="1.498292" y3="0.092734" z3="1.344294"/>
        <atom id="a10" elementType="H" x3="-0.212315" y3="1.161486" z3="2.615580"/>
        <atom id="a11" elementType="H" x3="-1.403041" y3="0.538671" z3="1.473380"/>
        <atom id="a12" elementType="H" x3="-0.570330" y3="-0.579104" z3="2.566987"/>
      </atomArray>
```

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<bondArray>
   <bond atomRefs2="a4 a3" order="1"/>
   <bond atomRefs2="a4 a7" order="1"/>
   <bond atomRefs2="a3 a1" order="1"/>
   <bond atomRefs2="a5 a1" order="1"/>
   <bond atomRefs2="a1 a6" order="1"/>
   <bond atomRefs2="a1 a2" order="1"/>
   <bond atomRefs2="a2 a9" order="1"/>
   <bond atomRefs2="a2 a8" order="1"/>
   <bond atomRefs2="a11 a8" order="1"/>
   <bond atomRefs2="a8 a12" order="1"/>
   <bond atomRefs2="a8 a10" order="1"/>
</bondArray>
<propertyList>
   <property title="Energy" dictRef="me:ZPE">
      <scalar units="kJ/mol" >-205.9</scalar>
   </property>
   <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
      <array units="cm-1">101.31 164.96 207.79 315.55 451.99 479.03 613.25 754.87 873.78
938.75 1050.02 1070.42 1154.26 1173.22 1230.95 1317.07 1408.78 1436.24 1461.22 1486.56
1498.62 1513.25 1531.48 2999.32 3010.65 3088.81 3099.11 3140.38 3580.64 3670.70 </array>
   </property>
   <property dictRef="me:epsilon">
      <scalar>216.11</scalar>
   </property>
   <property dictRef="me:sigma">
      <scalar>4.6</scalar>
   </property>
   <property title="Symmetry Number" dictRef="me:symmetryNumber">
      <scalar> 3 </scalar>
   </property>
</propertyList>
<me:energyTransferModel xsi:type="me:ExponentialDown">
```

```
        <me:deltaEDown units="cm-1">200.0</me:deltaEDown>
      </me:energyTransferModel>
      <me:DOSCMethod xsi:type="QMRotors"/>
    </molecule>
  </moleculeList>
  <reactionList>

    <reaction id="R_1">
      <reactant>
        <molecule ref="NH2CH3"  role="excessReactant" />
      </reactant>
      <reactant>
        <molecule ref="Criegee"  role="deficientReactant" />
      </reactant>
      <product>
        <molecule ref="complex"  role="modelled" />
      </product>
      <me:MCRCMethod xsi:type="MesmerILT">
        <me:preExponential>1.00e-10</me:preExponential>
        <me:activationEnergy  units="cm-1" >0</me:activationEnergy>
        <me:nInfinity>0.0</me:nInfinity>
      </me:MCRCMethod>
      <me:excessReactantConc>1.0E15</me:excessReactantConc>
    </reaction>
    <reaction id="R_2">
      <reactant>
        <molecule ref="complex" role="modelled" />
      </reactant>
      <product>
        <molecule ref="Prod" role="sink" />
      </product>
      <me:transitionState>
```

```
            <molecule ref="ts" role="transitionState" />
          </me:transitionState>
          <me:MCRCMethod name="SimpleRRKM"/>
        </reaction>



    </reactionList>

    <me:conditions>
      <me:bathGas>N2</me:bathGas>
      <me:PTs>
        <!-- <me:PTpair units="Torr" P="10" T="263"><me:experimentalEigenvalue EigenvalueID="1"
error="660">6640</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="10" T="267.4"><me:experimentalEigenvalue EigenvalueID="1"
error="600">6610</me:experimentalEigenvalue></me:PTpair>

        <me:PTpair units="Torr" P="10" T="275.8"><me:experimentalEigenvalue EigenvalueID="1"
error="1010">6350</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="10" T="288.5"><me:experimentalEigenvalue EigenvalueID="1"
error="340">5520</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="10" T="297.5"><me:experimentalEigenvalue EigenvalueID="1"
error="700">4410</me:experimentalEigenvalue></me:PTpair>-->
        <me:PTpair units="Torr" P="10" T="311.2"><me:experimentalEigenvalue EigenvalueID="1"
error="640">3600</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="50" T="258.2"><me:experimentalEigenvalue EigenvalueID="1"
error="800">7400</me:experimentalEigenvalue></me:PTpair>
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EigenvalueID="1" error="610">5960</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="50" T="275.6"><me:experimentalEigenvalue EigenvalueID="1"
error="1710">5130</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="50" T="284.4"><me:experimentalEigenvalue EigenvalueID="1"
error="1280">5340</me:experimentalEigenvalue></me:PTpair>
        <me:PTpair units="Torr" P="50" T="293.6"><me:experimentalEigenvalue EigenvalueID="1"
error="290">4740</me:experimentalEigenvalue></me:PTpair>
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```

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        <me:PTpair units="Torr" P="10" T="293"><me:experimentalEigenvalue EigenvalueID="1"
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        <me:PTpair units="Torr" P="20" T="293"><me:experimentalEigenvalue EigenvalueID="1"
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        <me:PTpair units="Torr" P="30" T="293"><me:experimentalEigenvalue EigenvalueID="1"
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        <me:PTpair units="Torr" P="60" T="293"><me:experimentalEigenvalue EigenvalueID="1"
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        <me:PTpair units="Torr" P="10" T="293"><me:experimentalEigenvalue EigenvalueID="1"
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      </me:PTs>

   </me:conditions>


   <me:modelParameters>

      <me:grainSize units="cm-1">25</me:grainSize>

      <me:energyAboveTheTopHill>10.</me:energyAboveTheTopHill>

   </me:modelParameters>


   <me:control>

     <!-- <me:calcMethod xsi:type="me:marquardt">

      <me:MarquardtIterations>10</me:MarquardtIterations>

      <me:MarquardtTolerance>0.1</me:MarquardtTolerance>

      <me:MarquardtDerivDelta>1.e-02</me:MarquardtDerivDelta>

      </me:calcMethod>-->

      <me:printSpeciesProfile/>

      <me:testRateConstants/>

      <me:printGrainedSpeciesProfile/>

      <me:eigenvalues>3</me:eigenvalues>

   </me:control>


</me:mesmer>
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