Kinetic data for MISTRA

supplemental material to:

S. Pechtl, E. R. Lovejoy, J. B. Burkholder, and R. von Glasow
Modeling the possible role of iodine oxides in atmospheric new particle formation
Atmos. Chem. Phys. Discuss., 2005

January 3, 2006
1 Tables of reaction rates

This collection comprises a complete listing of all gas and aqueous phase species (Table 1), gas phase (Table 2) and aqueous phase (Table 3) reaction rates, as well as rates for the heterogeneous (particle surface) reactions (Table 4), aqueous phase equilibrium constants (Table 5), Henry constants and accommodations coefficients (Table 6).

<table>
<thead>
<tr>
<th>Table 1: Species</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Gas phase</strong></td>
</tr>
<tr>
<td>O\textsuperscript{1}D, O\textsubscript{2}, O\textsubscript{3}, OH, HO\textsubscript{2}, H\textsubscript{2}O\textsubscript{2}, H\textsubscript{2}O</td>
</tr>
<tr>
<td>NO, NO\textsubscript{2}, NO\textsubscript{3}, N\textsubscript{2}O\textsubscript{5}, HONO, HNO\textsubscript{3}, HNO\textsubscript{4}, PAN, NH\textsubscript{3}</td>
</tr>
<tr>
<td>CO, CO\textsubscript{2}, CH\textsubscript{4}, C\textsubscript{2}H\textsubscript{6}, C\textsubscript{2}H\textsubscript{4}, HCHO, HCOOH, HCO, HCHO, HCOOH, ALD (i.e., CH\textsubscript{3}CHO), CH\textsubscript{2}O\textsubscript{2}, HCHO, H\textsubscript{2}O\textsubscript{2}, CH\textsubscript{3}CO\textsubscript{3}, CH\textsubscript{2}O\textsubscript{2}, C\textsubscript{2}H\textsubscript{5}O\textsubscript{2}, CH\textsubscript{3}O\textsubscript{2}, EO (i.e., CH\textsubscript{3}CHO), CH\textsubscript{2}O\textsubscript{2}, ROOH (i.e., alkylhydroperoxides)</td>
</tr>
<tr>
<td>SO\textsubscript{2}, SO\textsubscript{3}, HOSO\textsubscript{2}, H\textsubscript{2}SO\textsubscript{4}, DMS, CH\textsubscript{3}SCH\textsubscript{2}OO, DMSO, DMSO\textsubscript{2}, CH\textsubscript{3}S, CH\textsubscript{3}SCH\textsubscript{2}O\textsubscript{2}, CH\textsubscript{3}SO\textsubscript{2}H, CH\textsubscript{3}SO\textsubscript{3}H</td>
</tr>
<tr>
<td>Cl, ClO, OCl\textsubscript{O}, HCl, HOCI, Cl\textsubscript{2}, Cl\textsubscript{2}O\textsubscript{2}, Cl\textsubscript{NO\textsubscript{2}}, Cl\textsubscript{NO\textsubscript{3}}</td>
</tr>
<tr>
<td>Br, BrO, HBr, HOB\textsubscript{r}, Br\textsubscript{2}, BrNO\textsubscript{2}, BrNO\textsubscript{3}, BrCl</td>
</tr>
<tr>
<td>I, IO, OIO, HI, HOI, INO\textsubscript{2}, INO\textsubscript{3}, I\textsubscript{2}, ICl, IBr, HI\textsubscript{O}3, CH\textsubscript{3}I, C\textsubscript{2}H\textsubscript{5}I, C\textsubscript{3}H\textsubscript{7}I, CH\textsubscript{2}Cl\textsubscript{2}, CH\textsubscript{2}Br\textsubscript{I}, CH\textsubscript{2}I\textsubscript{2}</td>
</tr>
<tr>
<td><strong>Liquid phase (neutral)</strong></td>
</tr>
<tr>
<td>O\textsubscript{2}, O\textsubscript{3}, OH, HO\textsubscript{2}, H\textsubscript{2}O\textsubscript{2}, H\textsubscript{2}O</td>
</tr>
<tr>
<td>NO, NO\textsubscript{2}, NO\textsubscript{3}, HONO, HNO\textsubscript{3}, HNO\textsubscript{4}, NH\textsubscript{3}</td>
</tr>
<tr>
<td>CO\textsubscript{2}, HCHO, HCOOH, CH\textsubscript{3}OH, CH\textsubscript{3}OO, CH\textsubscript{3}OOH,DOM</td>
</tr>
<tr>
<td>SO\textsubscript{2}, H\textsubscript{2}SO\textsubscript{4}, DMSO, DMSO\textsubscript{2}, CH\textsubscript{3}SO\textsubscript{2}H, CH\textsubscript{3}SO\textsubscript{3}H</td>
</tr>
<tr>
<td>Cl, HCl, HOCI, Cl\textsubscript{2}</td>
</tr>
<tr>
<td>Br, HBr, HOB\textsubscript{r}, Br\textsubscript{2}, BrCl</td>
</tr>
<tr>
<td>IO, HI, HOI, I\textsubscript{2}, ICl, IBr</td>
</tr>
<tr>
<td><strong>Liquid phase (ions)</strong></td>
</tr>
<tr>
<td>H\textsuperscript{+}, OH\textsuperscript{−}, O\textsuperscript{2}</td>
</tr>
<tr>
<td>NO\textsubscript{2}, NO\textsubscript{3}, NO\textsubscript{4}, NH\textsuperscript{+}</td>
</tr>
<tr>
<td>HCO\textsuperscript{−}, CO\textsuperscript{−}, HCOO\textsuperscript{−}</td>
</tr>
<tr>
<td>HSO\textsuperscript{−}, SO\textsuperscript{2}−, HSO\textsubscript{4}−, SO\textsubscript{4}−, SO\textsubscript{3}−, SO\textsubscript{5}−, CH\textsubscript{3}SO\textsubscript{3}−, CH\textsubscript{2}OHSO\textsubscript{2}−, CH\textsubscript{2}OHSO\textsubscript{3}−</td>
</tr>
<tr>
<td>Cl\textsuperscript{−}, Cl\textsubscript{2}, ClO\textsuperscript{−}, ClOH\textsuperscript{−}</td>
</tr>
<tr>
<td>Br\textsuperscript{−}, Br\textsubscript{2}, BrO\textsuperscript{−}, BrCl\textsubscript{2}, Br\textsubscript{3}Cl\textsuperscript{−}, BrOH\textsuperscript{−}</td>
</tr>
<tr>
<td>I\textsuperscript{−}, IO\textsubscript{2}, IO\textsubscript{3}, ICl\textsubscript{2}, IBr\textsubscript{2}, ICl\textsubscript{Br}−</td>
</tr>
</tbody>
</table>
Table 2: Gas phase reactions.

<table>
<thead>
<tr>
<th>no</th>
<th>reaction</th>
<th>( n )</th>
<th>( A ) [(cm(^{-3})](^{1-n_s^{-1}})]</th>
<th>(-E_a ) / ( R ) [K]</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>O 1</td>
<td>O(^{1}D) + O(_2) (\rightarrow) O(_3)</td>
<td>2</td>
<td>(3.2 \times 10^{-11})</td>
<td>70</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 2</td>
<td>O(^{1}D) + N(_2) (\rightarrow) O(_3)</td>
<td>2</td>
<td>(1.8 \times 10^{-11})</td>
<td>110</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 3</td>
<td>O(^{1}D) + H(_2)O (\rightarrow) 2 OH</td>
<td>2</td>
<td>(2.2 \times 10^{-10})</td>
<td>110</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 4</td>
<td>OH + O(_3) (\rightarrow) HO(_2) + O(_2)</td>
<td>2</td>
<td>(1.7 \times 10^{-12})</td>
<td>-940</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 5</td>
<td>OH + HO(_2) (\rightarrow) H(_2)O + O(_2)</td>
<td>2</td>
<td>(4.8 \times 10^{-11})</td>
<td>250</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 6</td>
<td>OH + H(_2)O(_2) (\rightarrow) HO(_2) + H(_2)O</td>
<td>2</td>
<td>(2.9 \times 10^{-12})</td>
<td>-160</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 7</td>
<td>HO(_2) + O(_3) (\rightarrow) OH + 2O(_2)</td>
<td>2</td>
<td>(1.0 \times 10^{-14})</td>
<td>-490</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 8</td>
<td>HO(_2) + HO(_2) (\rightarrow) H(_2)O(_2) + O(_2)</td>
<td>2</td>
<td>(2.3 \times 10^{-13})</td>
<td>600</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>O 9</td>
<td>O(_3) + h\nu (\rightarrow) O(_2) + O(^{1}D)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>O 10</td>
<td>H(_2)O(_2) + h\nu (\rightarrow) 2OH</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 1</td>
<td>NO + OH (\rightarrow) HONO</td>
<td>3</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 2</td>
<td>NO + HO(_2) (\rightarrow) NO(_2) + OH</td>
<td>2</td>
<td>(3.5 \times 10^{-12})</td>
<td>250</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>N 3</td>
<td>NO + O(_3) (\rightarrow) NO(_2) + O(_2)</td>
<td>2</td>
<td>(3.0 \times 10^{-12})</td>
<td>-1500</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 4</td>
<td>NO + NO(_3) (\rightarrow) 2NO(_2)</td>
<td>2</td>
<td>(1.5 \times 10^{-11})</td>
<td>-1500</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 5</td>
<td>NO(_2) + OH (\rightarrow) HNO(_3)</td>
<td>3</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 6</td>
<td>NO(_2) + HO(_2) (\rightarrow) HNO(_4)</td>
<td>3</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 7</td>
<td>NO(_2) + O(_3) (\rightarrow) NO(_3) + O(_2)</td>
<td>2</td>
<td>(1.2 \times 10^{-13})</td>
<td>-2450</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 8</td>
<td>NO(_2) + h\nu (\rightarrow) NO + O(_3)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 9</td>
<td>NO(_2) + NO(_3) (\rightarrow) N(_2)O(_5)</td>
<td>3</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 10</td>
<td>NO(_2) + h\nu (\rightarrow) NO + O(_2)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Wayne et al. (1991)</td>
</tr>
<tr>
<td>N 11</td>
<td>NO(_3) + HO(_2) (\rightarrow) 0.3 HNO(_3) + 0.7 OH + 0.7 NO(_2) + O(_2)</td>
<td>2</td>
<td>(4.0 \times 10^{-12})</td>
<td></td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>N 12</td>
<td>NO(_3) + NO(_3) (\rightarrow) NO(_2) + NO(_2) + O(_2)</td>
<td>2</td>
<td>(8.5 \times 10^{-13})</td>
<td>-2450</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 13</td>
<td>NO(_3) + h\nu (\rightarrow) NO(_2) + O(_3)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Wayne et al. (1991)</td>
</tr>
<tr>
<td>N 14</td>
<td>N(_2)O(_5) (\rightarrow) NO(_2) + NO(_3)</td>
<td>2</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 15</td>
<td>N(_2)O(_5) + H(_2)O (\rightarrow) 2HNO(_3)</td>
<td>2</td>
<td>(2.6 \times 10^{-22})</td>
<td></td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>N 16</td>
<td>N(_2)O(_5) + h\nu (\rightarrow) NO(_2) + NO(_3)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 17</td>
<td>HONO + OH (\rightarrow) NO(_2)</td>
<td>2</td>
<td>(1.8 \times 10^{-11})</td>
<td>-390</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 18</td>
<td>HONO + h\nu (\rightarrow) NO + OH</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 19</td>
<td>HNO(_3) + h\nu (\rightarrow) NO(_2) + OH</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 20</td>
<td>HNO(_3) + OH (\rightarrow) NO(_3) + H(_2)O</td>
<td>2</td>
<td>2</td>
<td></td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>N 21</td>
<td>HNO(_4) (\rightarrow) NO(_2) + HO(_2)</td>
<td>2</td>
<td>2</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>N 22</td>
<td>HNO(_4) + OH (\rightarrow) NO(_2) + H(_2)O + O(_2)</td>
<td>2</td>
<td>(1.3 \times 10^{-12})</td>
<td>380</td>
<td>Haggerstone et al. (2005)</td>
</tr>
<tr>
<td>N 23</td>
<td>HNO(_4) + h\nu (\rightarrow) NO(_2) + HO(_2)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>N 24</td>
<td>HNO(_4) + h\nu (\rightarrow) OH + NO(_3)</td>
<td>1</td>
<td>1</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>no</td>
<td>reaction</td>
<td>$n$</td>
<td>$A \ [\text{cm}^{-3}1^{-n_S-1}]$</td>
<td>$-E_a / R \ [\text{K}]$</td>
<td>reference</td>
</tr>
<tr>
<td>----</td>
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<td>--------------------------------</td>
<td>----------------------------</td>
<td>-----------</td>
</tr>
<tr>
<td>C 1</td>
<td>CO + OH $\overset{O_2}{\rightarrow}$ HO$_2$ + CO$_2$</td>
<td>2</td>
<td>2</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 2</td>
<td>CH$_4$ + OH $\overset{O_2}{\rightarrow}$ CH$_3$OO + H$_2$O</td>
<td>2</td>
<td>2.4×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 3</td>
<td>C$_2$H$_6$ + OH $\rightarrow$ C$_2$H$_5$O$_2$ + H$_2$O</td>
<td>2</td>
<td>1.7×10$^{-11}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 4</td>
<td>C$_2$H$_4$ + OH $\rightarrow$ EO$_2$</td>
<td>2</td>
<td>1.66×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 5</td>
<td>C$_2$H$_4$ + O$_3$ $\rightarrow$ HCHO + 0.4CH$_2$O$_2$ + 0.12HO$_2$ + 0.42CO + 0.06CH$_4$</td>
<td>2</td>
<td>1.2×10$^{-14}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 6</td>
<td>HO$_2$ + CH$_3$OO $\rightarrow$ ROOH + O$_2$</td>
<td>2</td>
<td>4.1×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 7</td>
<td>HO$_2$ + C$_2$H$_5$O$_2$ $\rightarrow$ ROOH + O$_2$</td>
<td>2</td>
<td>7.5×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 8</td>
<td>HO$_2$ + CH$_3$CO$_2$ $\rightarrow$ ROOH + O$_2$</td>
<td>2</td>
<td>4.5×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 9</td>
<td>CH$_3$OO + CH$_3$OO $\rightarrow$ 1.4HCHO + 0.8HO$_2$ + O$_2$</td>
<td>2</td>
<td>1.5×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 10</td>
<td>C$_2$H$_5$O$_2$ + NO $\rightarrow$ ALD + HO$_2$ + NO$_2$</td>
<td>2</td>
<td>4.2×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 11</td>
<td>2C$_2$H$_5$O$_2$ $\rightarrow$ 1.6ALD + 1.2HO$_2$</td>
<td>2</td>
<td>5.0×10$^{-14}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 12</td>
<td>EO$_2$ + NO $\rightarrow$ NO$_2$ + 2.0HCHO + HO$_2$</td>
<td>2</td>
<td>4.2×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 13</td>
<td>EO$_2$ + EO$_2$ $\rightarrow$ 2.4HCHO + 1.2HO$_2$ + 0.4ALD</td>
<td>2</td>
<td>5.0×10$^{-14}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 14</td>
<td>HO$_2$ + EO$_2$ $\rightarrow$ ROOH + O$_2$</td>
<td>2</td>
<td>3.0×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 15</td>
<td>HCHO + $h\nu$ $\rightarrow$ 2HO$_2$ + CO</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C 16</td>
<td>HCHO + $h\nu$ $\rightarrow$ CO + H$_2$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C 17</td>
<td>HCHO + OH $\overset{O_2}{\rightarrow}$ HO$_2$ + CO + H$_2$O</td>
<td>2</td>
<td>1.00×10$^{-11}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 18</td>
<td>HCHO + HO$_2$ $\rightarrow$ HOCH$_2$O$_2$</td>
<td>2</td>
<td>6.7×10$^{-15}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 19</td>
<td>HCHO + NO$_3$ $\overset{O_2}{\rightarrow}$ HNO$_4$ + HO$_2$ + CO</td>
<td>2</td>
<td>5.8×10$^{-16}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 20</td>
<td>ALD + OH $\rightarrow$ CH$_3$CO$_2$ + H$_2$O</td>
<td>2</td>
<td>6.9×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 21</td>
<td>ALD + NO$_3$ $\rightarrow$ HNO$_3$ + CH$_3$CO$_2$</td>
<td>2</td>
<td>1.40×10$^{-15}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 22</td>
<td>ALD + $h\nu$ $\rightarrow$ CH$_3$OO + HO$_2$ + CO</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C 23</td>
<td>ALD + $h\nu$ $\rightarrow$ CH$_4$ + CO</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C 24</td>
<td>HOCH$_2$O$_2$ + NO $\rightarrow$ HCOOH + HO$_2$ + NO$_2$</td>
<td>2</td>
<td>4.2×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 25</td>
<td>HOCH$_2$O$_2$ + HO$_2$ $\rightarrow$ HCOOH + H$_2$O + O$_2$</td>
<td>2</td>
<td>2.00×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 26</td>
<td>2 HOCH$_2$O$_2$ $\rightarrow$ 2HCOOH + 2HO$_2$ + 2O$_2$</td>
<td>2</td>
<td>1.00×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 27</td>
<td>HCOOH + OH $\overset{O_2}{\rightarrow}$ HO$_2$ + H$_2$O + CO$_2$</td>
<td>2</td>
<td>4.0×10$^{-13}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 28</td>
<td>CH$_3$CO$_3$ + NO$_2$ $\rightarrow$ PAN</td>
<td>2</td>
<td>4.70×10$^{-12}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 29</td>
<td>PAN $\rightarrow$ CH$_3$CO$_3$ + NO$_2$</td>
<td>1</td>
<td>1.9×10$^{16}$</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>C 30</td>
<td>CH$_3$CO$_3$ + NO $\rightarrow$ CH$_3$OO + NO$_2$ + CO$_2$</td>
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<td>(1.6 \times 10^{-12})</td>
<td>1</td>
<td>Aranda et al. (1997)</td>
</tr>
<tr>
<td>Br 11</td>
<td>(\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{Br} + \text{HCHO} + \text{HO}_2)</td>
<td>2</td>
<td>(1.5 \times 10^{-14})</td>
<td>1</td>
<td>Hansen et al. (1999)</td>
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<tr>
<td>Br 12</td>
<td>(\text{BrO} + \text{HCHO} + \text{O}_2 \rightarrow \text{HOBr} + \text{CO} + \text{HO}_2)</td>
<td>2</td>
<td>(8.7 \times 10^{-12})</td>
<td>260</td>
<td>Orlando et al. (2004)</td>
</tr>
<tr>
<td>Br 13</td>
<td>(\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2)</td>
<td>2</td>
<td>(2.4 \times 10^{-12})</td>
<td>40</td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>Br 14</td>
<td>(\text{BrO} + \text{NO}_2 + \text{M} \rightarrow \text{BrNO}_3)</td>
<td>3</td>
<td>(2.9 \times 10^{-14})</td>
<td>860</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Br 15</td>
<td>(\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2)</td>
<td>2</td>
<td>(5.5 \times 10^{-12})</td>
<td>205</td>
<td>Orlando and Tyndall (1996)</td>
</tr>
<tr>
<td>Br 16</td>
<td>(\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2)</td>
<td>2</td>
<td>(1.1 \times 10^{-12})</td>
<td>205</td>
<td>Orlando and Tyndall (1996)</td>
</tr>
<tr>
<td>Br 17</td>
<td>(\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{Br} + \text{H}_2\text{O})</td>
<td>1</td>
<td>(1.1 \times 10^{-12})</td>
<td>205</td>
<td>Orlando and Tyndall (1996)</td>
</tr>
<tr>
<td>Br 18</td>
<td>(\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2)</td>
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<td>(1.1 \times 10^{-12})</td>
<td>205</td>
<td>Orlando and Tyndall (1996)</td>
</tr>
<tr>
<td>no</td>
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<td>$A \text{[cm}^{-3}\text{s}^{-1}]$</td>
<td>$-E_a / R \text{[K]}$</td>
<td>reference</td>
</tr>
<tr>
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<td>--------------------------</td>
<td>----------------</td>
<td>---------</td>
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<tr>
<td>11</td>
<td>$I + O_3 \rightarrow IO + O_2$</td>
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<td>$1.9 \times 10^{-11}$</td>
<td>-830</td>
<td>Atkinson et al. (2004)</td>
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<tr>
<td>12</td>
<td>$I + HO_2 \rightarrow HI + O_2$</td>
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<td>$1.5 \times 10^{-11}$</td>
<td>-1090</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>13</td>
<td>$I + NO_2 \rightarrow INO_2$</td>
<td>3</td>
<td>2</td>
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<tr>
<td>14</td>
<td>$I + NO_3 \rightarrow IO + NO_2$</td>
<td>2</td>
<td>$4.5 \times 10^{-10}$</td>
<td></td>
<td>Chambers et al. (1992)</td>
</tr>
<tr>
<td>15</td>
<td>$I + I \rightarrow I_2$</td>
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<td>$2.99 \times 10^{-11}$</td>
<td></td>
<td>Hippler et al. (1973)</td>
</tr>
<tr>
<td>16</td>
<td>$IO + HO_2 \rightarrow HOI + O_2$</td>
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<td>$1.4 \times 10^{-11}$</td>
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<td>Atkinson et al. (2004)</td>
</tr>
<tr>
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<td>$IO + NO \rightarrow I + NO_2$</td>
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<td>$7.15 \times 10^{-12}$</td>
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<td>Atkinson et al. (2004)</td>
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<tr>
<td>18</td>
<td>$IO + NO_2 \rightarrow INO_3$</td>
<td>3</td>
<td>2</td>
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<td></td>
</tr>
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<td>Atkinson et al. (2004), for product ratios see text</td>
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<tr>
<td>20</td>
<td>$OIO + OH \rightarrow 0.5 \text{HIO}_3 + 0.5 \text{HOI}$</td>
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<td>$2.0 \times 10^{-10}$</td>
<td></td>
<td>assumed, see von Glasow et al. (2002b)</td>
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<td>21</td>
<td>$OIO + NO \rightarrow \text{NO}_3 + IO$</td>
<td>2</td>
<td>$5.1 \times 10^{-13}$</td>
<td>712</td>
<td>THALOZ (2005)</td>
</tr>
<tr>
<td>22</td>
<td>$HI + OH \rightarrow I + H_2O$</td>
<td>2</td>
<td>$1.6 \times 10^{-11}$</td>
<td>440</td>
<td>Atkinson et al. (2004)</td>
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<tr>
<td>23</td>
<td>$HI + NO_3 \rightarrow I + HNO_3$</td>
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<td>-1830</td>
<td>Atkinson et al. (2004)</td>
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<td>24</td>
<td>$INO_2 \rightarrow I + NO_2$</td>
<td>2</td>
<td>2.4</td>
<td></td>
<td>estimated from data in Jenkin et al. (1985)</td>
</tr>
<tr>
<td>25</td>
<td>$INO_3 \rightarrow IO + NO_2$</td>
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<td>$1.1 \times 10^{15}$</td>
<td>-12060</td>
<td>Atkinson et al. (2005)</td>
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<tr>
<td>26</td>
<td>$I_2 + OH \rightarrow I + HOI$</td>
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<td>$2.1 \times 10^{-10}$</td>
<td></td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>27</td>
<td>$I_2 + NO_3 \rightarrow I + INO_3$</td>
<td>2</td>
<td>$1.5 \times 10^{-12}$</td>
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<td>Chambers et al. (1992)</td>
</tr>
<tr>
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<td>$CH_3I + OH \rightarrow HCHO + I$</td>
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<td>$4.3 \times 10^{-12}$</td>
<td>-1120</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>29</td>
<td>$C_3H_7I + OH \rightarrow CH_3OO + I$</td>
<td>2</td>
<td>$1.2 \times 10^{-12}$</td>
<td></td>
<td>J. Crowley, pers. comm.</td>
</tr>
<tr>
<td>30</td>
<td>$IO + h\nu \rightarrow O_2 + I + O_3$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Laszlo et al. (1995)</td>
</tr>
<tr>
<td>31</td>
<td>$OIO + h\nu \rightarrow I + O_2$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>THALOZ (2005), for sensitivity studies see text</td>
</tr>
<tr>
<td>32</td>
<td>$HOI + h\nu \rightarrow I + OH$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Bauer et al. (1998)</td>
</tr>
<tr>
<td>33</td>
<td>$INO_2 + h\nu \rightarrow I + NO_2$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Bröské and Zabel (1998) , R. Bröské, pers. comm.</td>
</tr>
<tr>
<td>34</td>
<td>$INO_3 + h\nu \rightarrow I + NO_3$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>same as BrNO_3, but redshifted by 50 um</td>
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<tr>
<td>35</td>
<td>$I_2 + h\nu \rightarrow 2I$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Wesely (1989)</td>
</tr>
<tr>
<td>36</td>
<td>$CH_3I + h\nu \rightarrow I + CH_3OO$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Roehl et al. (1997)</td>
</tr>
<tr>
<td>37</td>
<td>$C_2H_5I + h\nu \rightarrow I + ROOH$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>$= CH_3I$</td>
</tr>
<tr>
<td>38</td>
<td>$C_3H_7I + h\nu \rightarrow I + ROOH$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Roehl et al. (1997)</td>
</tr>
<tr>
<td>39</td>
<td>$CH_2Cl + h\nu \rightarrow I + Cl + 2HO_2 + CO$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Roehl et al. (1997)</td>
</tr>
<tr>
<td>40</td>
<td>$CH_2BrI + h\nu \rightarrow I + Br + 2HO_2 + CO$</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Mösinger et al. (1998)</td>
</tr>
<tr>
<td>41</td>
<td>$CH_2I_2 + h\nu \rightarrow I + IO + HCHO$</td>
<td>1</td>
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<td>Roehl et al. (1997)</td>
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</table>
Table 2: Continued.

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<tr>
<th>no</th>
<th>reaction</th>
<th>(n)</th>
<th>(A) ([\text{cm}^{-3}]^{1-nS^{-1}})</th>
<th>(-E_a/R) [K]</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hx 1</td>
<td>(\text{Cl} + \text{CH}_3\text{I} \rightarrow \text{HCl} + \text{HCHO} + \text{I})</td>
<td>2</td>
<td>(2.9 \times 10^{-11})</td>
<td>-1000</td>
<td>Sander et al. (2003), products simplified</td>
</tr>
<tr>
<td>Hx 2</td>
<td>(\text{Cl} + \text{BrCl} \rightarrow \text{Br} + \text{Cl}_2)</td>
<td>2</td>
<td>(1.5 \times 10^{-11})</td>
<td></td>
<td>Mallard et al. (1993)</td>
</tr>
<tr>
<td>Hx 3</td>
<td>(\text{Cl} + \text{Br}_2 \rightarrow \text{BrCl} + \text{Br})</td>
<td>2</td>
<td>(1.2 \times 10^{-10})</td>
<td></td>
<td>Mallard et al. (1993)</td>
</tr>
<tr>
<td>Hx 4</td>
<td>(\text{I}_2 + \text{Cl} \rightarrow \text{I} + \text{ICl})</td>
<td>2</td>
<td>(2.09 \times 10^{-10})</td>
<td></td>
<td>Bedjanian et al. (1996)</td>
</tr>
<tr>
<td>Hx 5</td>
<td>(\text{Br} + \text{OClO} \rightarrow \text{BrO} + \text{ClO})</td>
<td>2</td>
<td>(2.6 \times 10^{-11})</td>
<td>-1300</td>
<td>Mallard et al. (2004)</td>
</tr>
<tr>
<td>Hx 6</td>
<td>(\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl})</td>
<td>2</td>
<td>(1.1 \times 10^{-15})</td>
<td></td>
<td>Mallard et al. (1993)</td>
</tr>
<tr>
<td>Hx 7</td>
<td>(\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl})</td>
<td>2</td>
<td>(3.3 \times 10^{-15})</td>
<td></td>
<td>Mallard et al. (1993)</td>
</tr>
<tr>
<td>Hx 8</td>
<td>(\text{I}_2 + \text{Br} \rightarrow \text{I} + \text{IBr})</td>
<td>2</td>
<td>(1.2 \times 10^{-10})</td>
<td></td>
<td>Bedjanian et al. (1997)</td>
</tr>
<tr>
<td>Hx 9</td>
<td>(\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br})</td>
<td>2</td>
<td>(1.2 \times 10^{-11})</td>
<td></td>
<td>Sander et al. (2003)</td>
</tr>
<tr>
<td>Hx 10</td>
<td>(\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OCIO})</td>
<td>2</td>
<td>(1.6 \times 10^{-12})</td>
<td>430</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Hx 11</td>
<td>(\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2)</td>
<td>2</td>
<td>(2.9 \times 10^{-12})</td>
<td>220</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Hx 12</td>
<td>(\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2)</td>
<td>2</td>
<td>(5.8 \times 10^{-13})</td>
<td>170</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Hx 13</td>
<td>(\text{IO} + \text{ClO} \rightarrow 0.8 \text{I} + 0.55 \text{OCIO} + 0.45 \text{O}_2 + 0.25 \text{Cl} + 0.2 \text{ICl})</td>
<td>2</td>
<td>(4.7 \times 10^{-12})</td>
<td>280</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Hx 14</td>
<td>(\text{IO} + \text{BrO} \rightarrow \text{Br} + 0.8 \text{OIO} + 0.2 \text{I} + 0.2 \text{O}_2)</td>
<td>2</td>
<td>(1.5 \times 10^{-11})</td>
<td>510</td>
<td>Atkinson et al. (2004)</td>
</tr>
<tr>
<td>Hx 15</td>
<td>(\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl})</td>
<td>1</td>
<td>(1)</td>
<td></td>
<td>DeMore et al. (1997)</td>
</tr>
<tr>
<td>Hx 16</td>
<td>(\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl})</td>
<td>1</td>
<td>(1)</td>
<td></td>
<td>Seery and Britton (1964)</td>
</tr>
<tr>
<td>Hx 17</td>
<td>(\text{IBr} + h\nu \rightarrow \text{I} + \text{Br})</td>
<td>1</td>
<td>(1)</td>
<td></td>
<td>Seery and Britton (1964)</td>
</tr>
</tbody>
</table>

\(n\) is the order of the reaction. \(^1\) photolysis rates calculated online, \(^2\) special rate functions (pressure dependent and/or humidity dependent). Notes: The rates for ROOH were assumed as that of \(\text{CH}_3\text{OOH}\); \(\text{C}_2\text{H}_4\) is used as generic alkene as in the Lurmann et al. (1986) mechanism. The rate coefficients are calculated with \(k = A \times \exp(-E_a/kT)\).
Table 3: Aqueous phase reactions.

<table>
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<th>no</th>
<th>reaction</th>
<th>n</th>
<th>$k_0 , ([M^{n-}]s^{-1})$</th>
<th>$-E_a / R [K]$</th>
<th>reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>O 1</td>
<td>$O_3 + OH \rightarrow HO_2$</td>
<td>2</td>
<td>$1.1 \times 10^8$</td>
<td>-</td>
<td>Sehested et al. (1984)</td>
</tr>
<tr>
<td>O 2</td>
<td>$O_3 + O_2 \rightarrow OH + OH^-$</td>
<td>2</td>
<td>$1.5 \times 10^9$</td>
<td>-</td>
<td>Sehested et al. (1983)</td>
</tr>
<tr>
<td>O 3</td>
<td>$OH + OH \rightarrow H_2O_2$</td>
<td>2</td>
<td>$5.5 \times 10^9$</td>
<td>-</td>
<td>Buxton et al. (1988)</td>
</tr>
<tr>
<td>O 4</td>
<td>$OH + HO_2 \rightarrow H_2O$</td>
<td>2</td>
<td>$7.1 \times 10^9$</td>
<td>-</td>
<td>Sehested et al. (1968)</td>
</tr>
<tr>
<td>O 5</td>
<td>$OH + O_2 \rightarrow OH^-$</td>
<td>2</td>
<td>$1.0 \times 10^{10}$</td>
<td>-</td>
<td>Sehested et al. (1968)</td>
</tr>
<tr>
<td>O 6</td>
<td>$OH + H_2O_2 \rightarrow HO_2$</td>
<td>2</td>
<td>$2.7 \times 10^7$</td>
<td>-1684</td>
<td>Christensen et al. (1982)</td>
</tr>
<tr>
<td>O 7</td>
<td>$HO_2 + HO_2 \rightarrow H_2O_2$</td>
<td>2</td>
<td>$9.7 \times 10^5$</td>
<td>-2500</td>
<td>Christensen and Sehested (1988)</td>
</tr>
<tr>
<td>O 8</td>
<td>$HO_2 + O_2 \rightarrow H_2O_2$</td>
<td>2</td>
<td>$1.0 \times 10^8$</td>
<td>-900</td>
<td>Christensen and Sehested (1988)</td>
</tr>
<tr>
<td>N 1</td>
<td>$HONO + OH \rightarrow NO_2$</td>
<td>2</td>
<td>$1.0 \times 10^9$</td>
<td>-</td>
<td>assumed =N7 Barker et al. (1970)</td>
</tr>
<tr>
<td>N 2</td>
<td>$HONO + H_2O_2 \rightarrow HNO_3$</td>
<td>3</td>
<td>$4.6 \times 10^3$</td>
<td>-6800</td>
<td>Damschen and Martin (1983)</td>
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<tr>
<td>N 3</td>
<td>$NO_3 + OH^- \rightarrow NO_3^- + OH$</td>
<td>2</td>
<td>$8.2 \times 10^7$</td>
<td>-2700</td>
<td>Exner et al. (1992)</td>
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<td>$NO_2 + NO_2 \rightarrow HNO_2 + HONO$</td>
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<td>$1.0 \times 10^8$</td>
<td>-</td>
<td>Lee and Schwartz (1981)</td>
</tr>
<tr>
<td>N 5</td>
<td>$NO_2 + HO_2 \rightarrow HNO_4$</td>
<td>2</td>
<td>$1.8 \times 10^9$</td>
<td>-</td>
<td>Warneck (1999)</td>
</tr>
<tr>
<td>N 6</td>
<td>$NO_2^- + O_3 \rightarrow NO_3^- + O_2$</td>
<td>2</td>
<td>$5.0 \times 10^5$</td>
<td>-6950</td>
<td>Damschen and Martin (1983)</td>
</tr>
<tr>
<td>N 7</td>
<td>$NO_2^- + OH^- \rightarrow NO_2 + OH^-$</td>
<td>2</td>
<td>$1.0 \times 10^{10}$</td>
<td>-</td>
<td>Barker et al. (1970)</td>
</tr>
<tr>
<td>N 8</td>
<td>$NO_4^- \rightarrow NO_2 + O_2$</td>
<td>1</td>
<td>$8.0 \times 10^{-1}$</td>
<td>-</td>
<td>Warneck (1999)</td>
</tr>
<tr>
<td>C 1</td>
<td>$HCHO + OH \rightarrow HCOOH + HO_2$</td>
<td>2</td>
<td>$7.7 \times 10^8$</td>
<td>-1020</td>
<td>Chin and Wine (1994)</td>
</tr>
<tr>
<td>C 2</td>
<td>$HCOOH + OH \rightarrow HO_2 + CO_2$</td>
<td>2</td>
<td>$1.1 \times 10^8$</td>
<td>-991</td>
<td>Chin and Wine (1994)</td>
</tr>
<tr>
<td>C 3</td>
<td>$HCOO^- + OH^- \rightarrow OH^- + HO_2 + CO_2$</td>
<td>2</td>
<td>$3.1 \times 10^9$</td>
<td>-1240</td>
<td>Chin and Wine (1994)</td>
</tr>
<tr>
<td>C 4</td>
<td>$CH_3OO + HO_2 \rightarrow CH_2OOH$</td>
<td>2</td>
<td>$4.3 \times 10^5$</td>
<td>-</td>
<td>estimated by Jacob (1986)</td>
</tr>
<tr>
<td>C 5</td>
<td>$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$</td>
<td>2</td>
<td>$5.0 \times 10^7$</td>
<td>-</td>
<td>estimated by Jacob (1986)</td>
</tr>
<tr>
<td>C 6</td>
<td>$CH_3OO + OH^- \rightarrow HCHO + HO_2$</td>
<td>2</td>
<td>$9.7 \times 10^8$</td>
<td>-</td>
<td>Buxton et al. (1988)</td>
</tr>
<tr>
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<td>$CH_3OOH + OH^- \rightarrow CH_3OO$</td>
<td>2</td>
<td>$2.7 \times 10^7$</td>
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<td>estimated by Jacob (1986)</td>
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<td>C 8</td>
<td>$CH_3OOH + OH^- \rightarrow CH_3OO$</td>
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<td>$CO_3^- + O_2^- \rightarrow HCOO_2^- + OH^-$</td>
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<td>-</td>
<td>Ross et al. (1992)</td>
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<tr>
<td>C 10</td>
<td>$CO_3^- + H_2O_2 \rightarrow HCOO^- + HO_2$</td>
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<td>Ross et al. (1992)</td>
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<td>$CO_3^- + HCOO^- \rightarrow HCOO_2^- + HCO_3^- + HO_2$</td>
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<td>-</td>
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<td>C 12</td>
<td>$HCOO_2^- + OH^- \rightarrow CO_3^-$</td>
<td>2</td>
<td>$8.5 \times 10^6$</td>
<td>-</td>
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<td>C 13</td>
<td>$DOM + OH \rightarrow HO_2$</td>
<td>2</td>
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<td>estimated by (C. Anastasio, pers. comm.) from Ross et al. (1998)</td>
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<td>-</td>
<td>upper limit D. Sedlak pers. comm. with R. Sander</td>
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<td>-</td>
<td>upper limit D. Sedlak pers. comm. with R. Sander</td>
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<td>Damschen and Martin (1983)</td>
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<td>Boyce and Hoffmann (1984)</td>
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<td>$\text{SO}_4^- + \text{OH}^- \rightarrow \text{HSO}_5^-$</td>
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<td>Huie and Neta (1987)</td>
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<td>$\text{DMS} + \text{OH} \rightarrow 0.5\text{CH}_3\text{SO}_3^- + 0.5\text{CH}_3\text{OO} + 0.5\text{H}_2\text{O} + \text{HCHO} + \text{H}^+$</td>
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<td>$\text{CH}_3\text{SO}_3^- + \text{OH} \rightarrow \text{CH}_3\text{SO}_3^- + \text{H}_2\text{O} - \text{O}_2$</td>
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<td>$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$</td>
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<td>Wu et al. (1980)</td>
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<td>Fortnum et al. (1960)</td>
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<td>$Cl^- + HOCl + H^+ \rightarrow Cl_2$</td>
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<td>Cl 16</td>
<td>$Cl_2^- + HO_2 \rightarrow Cl^- + Cl^- + H^+ + O_2$</td>
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<td>$3.1 \times 10^9$</td>
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<td>$Cl_2^- + O_2 \rightarrow Cl^- + Cl^- + O_2$</td>
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<td>Jacobi et al. (1996)</td>
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<td>Cl 24</td>
<td>$Cl_2^- + Cl_2 \rightarrow Cl_2 + 2Cl^-$</td>
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<td>Yu (2001)</td>
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<tr>
<td>Cl 25</td>
<td>$Cl^- + Cl \rightarrow Cl^- + Cl_2$</td>
<td>2</td>
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<td>$6.0 \times 10^9$</td>
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<td>Yu (2001)</td>
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<td>$ClO^- + H^+ \rightarrow Cl^-$</td>
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<td>Cl 29</td>
<td>$HOCl + HO_2 \rightarrow Cl + O_2$</td>
<td>2</td>
<td>$7.5 \times 10^6$</td>
<td>-</td>
<td>assumed = Cl30 Long and Bielski (1980)</td>
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<td>$HOCl + O_2^- \rightarrow Cl + OH^- + O_2$</td>
<td>2</td>
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<td>-</td>
<td>Long and Bielski (1980)</td>
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<td>Cl 32</td>
<td>$HOCl + HSO_4^- \rightarrow Cl^- + HSO_4^- + H^+$</td>
<td>2</td>
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<td>Cl 33</td>
<td>$Cl_2 + HO_2 \rightarrow Cl_2 + H^+ + O_2$</td>
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<td>-</td>
<td>Bjergbakke et al. (1981)</td>
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<td>Cl 34</td>
<td>$Cl_2 + O_2^- \rightarrow Cl_2 + O_2$</td>
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<td>-</td>
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<td>$-E_a / R , \text{K}$</td>
<td>reference</td>
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<td>---------------------------------</td>
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<td>$\text{Br} + \text{OH}^- \rightarrow \text{BrOH}^-$</td>
<td>2</td>
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<td>Zehavi and Rabani (1972)</td>
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<tr>
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<td>Br 12</td>
<td>$\text{Br}_2 + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{HO}_2$</td>
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<td>estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)</td>
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<tr>
<td>Br 16</td>
<td>$\text{Br}_2^- + \text{NO}_2^- \rightarrow \text{Br}^- + \text{Br}^- + \text{NO}_2$</td>
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<td>$-1720$</td>
<td>Shoute et al. (1991)</td>
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<td>Br 17</td>
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<td>Br 19</td>
<td>$\text{Br}_2^- + \text{DMS} \rightarrow 0.5 \text{CH}_3\text{SO}_3^- + 0.5 \text{CH}_3\text{OO} + 0.5 \text{HSO}_4^- + \text{HCHO} + 2 \text{Br}^- + 2 \text{H}^+$</td>
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<td>Zehavi and Rabani (1972)</td>
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<td>Zehavi and Rabani (1972)</td>
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<td>Br 22</td>
<td>$\text{BrOH}^- + \text{H}^+ \rightarrow \text{Br}^- + \text{H}_2\text{O}$</td>
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<td>Zehavi and Rabani (1972)</td>
</tr>
<tr>
<td>Br 23</td>
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<td>Zehavi and Rabani (1972)</td>
</tr>
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<td>Br 24</td>
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<td></td>
<td>Troy and Margerum (1991)</td>
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<tr>
<td>Br 25</td>
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<td>Herrmann et al. (1999)</td>
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<td>Br 26</td>
<td>$\text{HOBr} + \text{O}_3^- \rightarrow \text{Br}^- + \text{OH}^- + \text{O}_2$</td>
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<td>Schwarz and Bielski (1986)</td>
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<td>Br 27</td>
<td>$\text{HOBr} + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{H}^+ + \text{O}_2$</td>
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<td>von Gunten and Oliveras (1998)</td>
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<td>Br 28</td>
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<td>Troy and Margerum (1991)</td>
</tr>
<tr>
<td>Br 29</td>
<td>$\text{HOBr} + \text{HSO}_4^- \rightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$</td>
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<td>Br 30</td>
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<td>2</td>
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<td></td>
<td>Ross et al. (1998)</td>
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<td>Br 31</td>
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<td>Ross et al. (1998)</td>
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### Table 3: Continued.

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<th>reference</th>
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<td>HOI + I$^-$ + H$^+$ $\rightarrow$ I$_2$</td>
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<td>$4.4 \times 10^{12}$</td>
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<td>Eigen and Kustin (1962)</td>
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<td>HOI + Cl$^-$ + H$^+$ $\rightarrow$ ICl</td>
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<td>$2.9 \times 10^{10}$</td>
<td></td>
<td>Wang et al. (1989)</td>
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<td>ICl $\rightarrow$ HOI + Cl$^-$ + H$^+$</td>
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<td></td>
<td>Wang et al. (1989)</td>
</tr>
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<td>HOI + Br$^-$ + H$^+$ $\rightarrow$ IBr</td>
<td>3</td>
<td>$3.3 \times 10^{12}$</td>
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<td>Troy et al. (1991)</td>
</tr>
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<td>IBr $\rightarrow$ HOI + H$^+$ + Br$^-$</td>
<td>1</td>
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<td>Troy et al. (1991)</td>
</tr>
<tr>
<td>6 I</td>
<td>HOCl + I$^-$ + H$^+$ $\rightarrow$ ICl</td>
<td>3</td>
<td>$3.5 \times 10^{11}$</td>
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<td>Nagy et al. (1988)</td>
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<td>HOBr + I$^-$ $\rightarrow$ IBr + OH$^-$</td>
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<td></td>
<td>Troy and Margerum (1991)</td>
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<td>8 I</td>
<td>IO$_2$ + H$_2$O$_2$ $\rightarrow$ IO$_3$</td>
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<td></td>
<td>Buxton et al. (1986)</td>
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<td>11 I</td>
<td>HOI + Cl$_2$ $\rightarrow$ IO$_2$ + 2Cl$^-$ + 3H$^+$</td>
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<td>Lengyel et al. (1996)</td>
</tr>
<tr>
<td>12 I</td>
<td>HOI + HOCl $\rightarrow$ IO$_2$ + Cl$^-$ + 2 H$^+$</td>
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<td></td>
<td>Citri and Epstein (1988)</td>
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<td></td>
<td>Chinake and Simoyi (1996)</td>
</tr>
<tr>
<td>14 I</td>
<td>IO$_2$ + HOCl $\rightarrow$ IO$_3$ + Cl$^-$ + H$^+$</td>
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<td>Lengyel et al. (1996)</td>
</tr>
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<td>IO$_2$ + HOBr $\rightarrow$ IO$_3$ + Br$^-$ + H$^+$</td>
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<td>Chinake and Simoyi (1996)</td>
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<td>16 I</td>
<td>IO$_2$ + HOI $\rightarrow$ IO$_3$ + I$^-$ + H$^+$</td>
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<td>Chinake and Simoyi (1996)</td>
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<tr>
<td>17 I</td>
<td>I$_2$ + HSO$_3$ $\rightarrow$ 2 I$^-$ + HSO$_2$ + 2 H$^+$</td>
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<td>Hx 1</td>
<td>Br$^-$ + HOCl + H$^+$ $\rightarrow$ BrCl</td>
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<td>Liu and Margerum (2001)</td>
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<td>Hx 2</td>
<td>Cl$^-$ + HOBr + H$^+$ $\rightarrow$ BrCl</td>
<td>3</td>
<td>$2.3 \times 10^{10}$</td>
<td></td>
<td>Liu and Margerum (2001)</td>
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<td>BrCl $\rightarrow$ Cl$^-$ + HOBr + H$^+$</td>
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<td>Liu and Margerum (2001)</td>
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<tr>
<td>Hx 4</td>
<td>Br$^-$ + ClO$^-$ + H$^+$ $\rightarrow$ BrCl + OH$^-$</td>
<td>3</td>
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<td>Kumar and Margerum (1987)</td>
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<td>Liu and Margerum (2001)</td>
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<td>BrCl$_2$ $\rightarrow$ Cl$_2$ + Br$^-$</td>
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<td>hv 1</td>
<td>O$_3$ + hv $\rightarrow$ OH + OH + O$_2$</td>
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<td>H$_2$O$_2$ + hv $\rightarrow$ OH + OH</td>
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<td>hv 3</td>
<td>NO$_3$ + hv $\rightarrow$ NO$_2$ + OH</td>
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<td>Zellner et al. (1990)</td>
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<td>NO$_2$ + hv $\rightarrow$ NO + OH</td>
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<td></td>
<td>Zellner et al. (1990); Burley and Johnston (1992)</td>
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<td>hv 7</td>
<td>HOBr + hv $\rightarrow$ OH + Br</td>
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<td>hv 8</td>
<td>Br$_2$ + hv $\rightarrow$ Br + Br</td>
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<td>hv 9</td>
<td>BrCl + hv $\rightarrow$ Cl + Br</td>
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<td>assumed 2x gas phase</td>
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$n$ is the order of the reaction. 1 photolysis rates calculated online. The temperature dependence is $k = k_0 \times \exp\left(\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, $T_0 = 298$ K.
Table 4: Heterogeneous reactions.

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<td>H 1</td>
<td>$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow \text{HNO}_3 + \text{HNO}_3$</td>
<td>$k_t(\text{N}_2\text{O}<em>5) w</em>{l,i}[\text{H}_2\text{O}]/\text{Het}_T$</td>
<td>Behnke et al. (1994), Behnke et al. (1997)</td>
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<tr>
<td>H 2</td>
<td>$\text{N}_2\text{O}_5 + \text{Cl}^- \rightarrow \text{ClNO}_2 + \text{NO}_3^-$</td>
<td>$k_t(\text{N}_2\text{O}<em>5) w</em>{l,i} f(\text{Cl}^-) [\text{Cl}^-]/\text{Het}_T$</td>
<td>Behnke et al. (1994), Behnke et al. (1997)</td>
</tr>
<tr>
<td>H 3</td>
<td>$\text{N}_2\text{O}_5 + \text{Br}^- \rightarrow \text{BrNO}_2 + \text{NO}_3^-$</td>
<td>$k_t(\text{N}_2\text{O}<em>5) w</em>{l,i} f(\text{Br}^-) [\text{Br}^-]/\text{Het}_T$</td>
<td>Behnke et al. (1994), Behnke et al. (1997)</td>
</tr>
<tr>
<td>H 4</td>
<td>$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCL}_aq + \text{HNO}_3$</td>
<td>$k_t(\text{ClNO}<em>3) w</em>{l,i} [\text{H}_2\text{O}]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 5</td>
<td>$\text{ClNO}_3 + \text{Cl}^- \rightarrow \text{Cl}_2 + \text{NO}_3^-$</td>
<td>$k_t(\text{ClNO}<em>3) w</em>{l,i} f(\text{Cl}^-) [\text{Cl}^-]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 6</td>
<td>$\text{ClNO}_3 + \text{Br}^- \rightarrow \text{BrCl}_aq + \text{NO}_3^-$</td>
<td>$k_t(\text{ClNO}<em>3) w</em>{l,i} f(\text{Br}^-) [\text{Br}^-]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 7</td>
<td>$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HBr}_aq + \text{HNO}_3$</td>
<td>$k_t(\text{BrNO}<em>3) w</em>{l,i} [\text{H}_2\text{O}]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 8</td>
<td>$\text{BrNO}_3 + \text{Cl}^- \rightarrow \text{BrCl}_aq + \text{NO}_3^-$</td>
<td>$k_t(\text{BrNO}<em>3) w</em>{l,i} f(\text{Cl}^-) [\text{Cl}^-]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 9</td>
<td>$\text{BrNO}_3 + \text{Br}^- \rightarrow \text{Br}_2 + \text{NO}_3^-$</td>
<td>$k_t(\text{BrNO}<em>3) w</em>{l,i} f(\text{Br}^-) [\text{Br}^-]/\text{Het}_T$</td>
<td>see note</td>
</tr>
<tr>
<td>H 10</td>
<td>$\text{INO}_3 + \text{H}_2\text{O} \rightarrow \text{HOI}_aq + \text{HNO}_3$</td>
<td>$k_t(\text{INO}<em>3) w</em>{l,i}$</td>
<td>assumed, see von Glasow et al. (2002b)</td>
</tr>
<tr>
<td>H 11</td>
<td>$\text{HI} + \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{I}^-$</td>
<td>$k_t(\text{HI}) w_{l,i}$</td>
<td>assumed, see von Glasow et al. (2002b)</td>
</tr>
<tr>
<td>H 12</td>
<td>$\text{INO}_2 + \text{H}_2\text{O} \rightarrow \text{HOI}_aq + \text{HNO}_aq$</td>
<td>$k_t(\text{INO}<em>2) w</em>{l,i}$</td>
<td>assumed, see von Glasow et al. (2002b)</td>
</tr>
<tr>
<td>H 13</td>
<td>$\text{OIO}_3 + \text{H}_2\text{O} \rightarrow \text{HOI}_aq + \text{HO}_aq$</td>
<td>$k_t(\text{OIO}<em>3) w</em>{l,i}$</td>
<td>assumed, see von Glasow et al. (2002b)</td>
</tr>
<tr>
<td>H 14</td>
<td>$\text{HOI} + \text{H}_2\text{O} \rightarrow \text{IO}^- + \text{H}^+$</td>
<td>$k_t(\text{HOI}) w_{l,i}$</td>
<td>assumed, see von Glasow et al. (2002b)</td>
</tr>
</tbody>
</table>

For a definition of $k_t$ and $w_{l,i}$ see von Glasow et al. (2002a) or von Glasow (2000). Het$_T = [\text{H}_2\text{O} + f(\text{Cl}^-) [\text{Cl}^-] + f(\text{Br}^-) [\text{Br}^-]]$, with $f(\text{Cl}^-) = 5.0 \times 10^2$ and $f(\text{Br}^-) = 3.0 \times 10^5$. H4 - H9: the total rate is determined by $k_t$, the distribution among the different reaction paths was assumed to be the same as for reactions H1 - H3.
### Table 5: Aqueous phase equilibrium constants.

<table>
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<th>no</th>
<th>reaction</th>
<th>$m$</th>
<th>$n$</th>
<th>$K_0$ [M$^{n-m}$]</th>
<th>$-\Delta H/R$ [K]</th>
<th>reference</th>
</tr>
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<tr>
<td>EQ 1</td>
<td>CO$_{2aq}$ $\rightleftharpoons$ H$^+$ + HCO$_3^-$</td>
<td>1</td>
<td>2</td>
<td>$4.3 \times 10^{-7}$</td>
<td>-913</td>
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<td>EQ 2</td>
<td>NH$_{3aq}$ $\rightleftharpoons$ OH$^-$ + NH$_4^+$</td>
<td>1</td>
<td>2</td>
<td>$1.7 \times 10^{-5}$</td>
<td>-4325</td>
<td>Chameides (1984)</td>
</tr>
<tr>
<td>EQ 3</td>
<td>H$<em>2$O$</em>{aq}$ $\rightleftharpoons$ H$^+$ + OH$^-$</td>
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<td>2</td>
<td>$1.0 \times 10^{-14}$</td>
<td>-6716</td>
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</tr>
<tr>
<td>EQ 4</td>
<td>HCOOH$_{aq}$ $\rightleftharpoons$ H$^+$ + HCOO$^-$</td>
<td>1</td>
<td>2</td>
<td>$1.8 \times 10^{-4}$</td>
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<td>Weast (1980)</td>
</tr>
<tr>
<td>EQ 5</td>
<td>HSO$_3^-$ $\rightleftharpoons$ H$^+$ + SO$_3^{2-}$</td>
<td>1</td>
<td>2</td>
<td>$6.0 \times 10^{-8}$</td>
<td>1120</td>
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<tr>
<td>EQ 6</td>
<td>H$_2$SO$_4aq$ $\rightleftharpoons$ H$^+$ + HSO$_4^-$</td>
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<td>Seinfeld and Pandis (1998)</td>
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<td>2</td>
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<td>Weast (1980)</td>
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<td>EQ 8</td>
<td>HO$_2$aq $\rightleftharpoons$ O$_2^-$ + H$^+$</td>
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<td>2</td>
<td>$1.6 \times 10^{-5}$</td>
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<td>EQ 9</td>
<td>SO$_2$aq $\rightleftharpoons$ H$^+$ + HS$_2$O$_3^-$</td>
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<td>2090</td>
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<td>Cl$<em>2$ $\rightleftharpoons$ Cl$</em>{aq}$ $+$ Cl$^-$</td>
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<td>2</td>
<td>$5.2 \times 10^{-6}$</td>
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<td>Jayson et al. (1973)</td>
</tr>
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<td>$3.2 \times 10^{-8}$</td>
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<td>EQ 12</td>
<td>HBr$_{aq}$ $\rightleftharpoons$ H$^+$ + Br$^-$</td>
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<td>Lax (1969)</td>
</tr>
<tr>
<td>EQ 13</td>
<td>Br$<em>2$ $\rightleftharpoons$ Br$</em>{aq}$ $+$ Br$^-$</td>
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<td>$9.1 \times 10^{-6}$</td>
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<td>Mamou et al. (1977)</td>
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<td>EQ 14</td>
<td>HOBr$_{aq}$ $\rightleftharpoons$ H$^+$ + BrO$^-$</td>
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<td>2</td>
<td>$2.3 \times 10^{-9}$</td>
<td>-3091</td>
<td>Kelley and Tartar (1956)</td>
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<td>EQ 15</td>
<td>BrCl$_{aq}$ + Cl$^-$ $\rightleftharpoons$ BrCl$_2$</td>
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<td>1</td>
<td>3.8</td>
<td>1143</td>
<td>Wang et al. (1994)</td>
</tr>
<tr>
<td>EQ 16</td>
<td>BrCl$_{aq}$ + Br$^-$ $\rightleftharpoons$ Br$_2$Cl$^-$</td>
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<td>1</td>
<td>$1.8 \times 10^{4}$</td>
<td></td>
<td>Wang et al. (1994)</td>
</tr>
<tr>
<td>EQ 17</td>
<td>Br$_{2aq}$ + Cl$^-$ $\rightleftharpoons$ Br$_2$Cl$^-$</td>
<td>2</td>
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<td>1.3</td>
<td></td>
<td>Wang et al. (1994)</td>
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<td>EQ 18</td>
<td>HNO$_3aq$ $\rightleftharpoons$ H$^+$ + NO$_3^-$</td>
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<td>$1.5 \times 10^{1}$</td>
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<td>Davis and de Bruin (1964)</td>
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<td>EQ 19</td>
<td>HCl$_{aq}$ $\rightleftharpoons$ H$^+$ + Cl$^-$</td>
<td>1</td>
<td>2</td>
<td>$1.7 \times 10^{6}$</td>
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<td>Marsh and McElroy (1985)</td>
</tr>
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<td>EQ 20</td>
<td>HONO$_{aq}$ $\rightleftharpoons$ H$^+$ + NO$_2^-$</td>
<td>1</td>
<td>2</td>
<td>$5.1 \times 10^{-4}$</td>
<td>-1260</td>
<td>Schwartz and White (1981)</td>
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<tr>
<td>EQ 21</td>
<td>HNO$_4aq$ $\rightleftharpoons$ NO$_4^-$ + H$^+$</td>
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<td>8700</td>
<td>Warneck (1999)</td>
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<td>EQ 22</td>
<td>ICl$_{aq}$ + Cl$^-$ $\rightleftharpoons$ ICl$_2$</td>
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<td>1</td>
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<td>Wang et al. (1989)</td>
</tr>
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<td>EQ 23</td>
<td>IBr$_{aq}$ + Br$^-$ $\rightleftharpoons$ IBr$_2$</td>
<td>2</td>
<td>1</td>
<td>$2.9 \times 10^{2}$</td>
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<td>Troy et al. (1991)</td>
</tr>
<tr>
<td>EQ 24</td>
<td>ICl$_{aq}$ + Br$^-$ $\rightleftharpoons$ IClBr$^-$</td>
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<td>EQ 25</td>
<td>IBr$_{aq}$ + Cl$^-$ $\rightleftharpoons$ IClBr$^-$</td>
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<td>1</td>
<td>1.3</td>
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<td>assumed = EQ 17</td>
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The temperature dependence is $K = K_0 \times \exp\left(\frac{-\Delta H}{R \cdot T}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, $T_0 = 298$ K.
<table>
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<th>$-\Delta_{solv}H/R$ [K]</th>
<th>reference</th>
<th>$\alpha^a$</th>
<th>$-\Delta_{obs}H/R$ [K]</th>
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<td>$1.2 \times 10^{-2}$</td>
<td>2560</td>
<td>Chameides (1984)</td>
<td>0.002</td>
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<td>DeMore et al. (1997)</td>
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<td>O$_2$</td>
<td>$1.3 \times 10^{-3}$</td>
<td>1500</td>
<td>Wilhelm et al. (1977)</td>
<td>0.01</td>
<td>2000</td>
<td>estimated</td>
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<td>OH</td>
<td>$3.0 \times 10^1$</td>
<td>4300</td>
<td>Hanson et al. (1992)</td>
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<td>Takami et al. (1998)</td>
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<td>HO$_2$</td>
<td>$3.9 \times 10^3$</td>
<td>5900</td>
<td>Hanson et al. (1992)</td>
<td>0.2</td>
<td>(at 293 K)</td>
<td>DeMore et al. (1997)</td>
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<td>H$_2$O$_2$</td>
<td>$1.0 \times 10^5$</td>
<td>6338</td>
<td>Lind and Kok (1994)</td>
<td>0.077</td>
<td>2769</td>
<td>Worsnop et al. (1989)</td>
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<td>2500</td>
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<td>0.0015</td>
<td>(at 298 K)</td>
<td>Ponche et al. (1993)</td>
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<td>NO$_3$</td>
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<td>2000</td>
<td>Thomas et al. (1993)</td>
<td>0.04</td>
<td>(at 273 K)</td>
<td>Rudich et al. (1996)</td>
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<td>N$_2$O$_5$</td>
<td>$\infty$</td>
<td>—</td>
<td>estimated</td>
<td>0.1</td>
<td>(at 195-300 K)</td>
<td>DeMore et al. (1997)</td>
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<td>HONO</td>
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<td>4780</td>
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<td>(at 247-297 K)</td>
<td>DeMore et al. (1997)</td>
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<td>HNO$_2$</td>
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<td>8694</td>
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<td>(at RT)</td>
<td>Abbatt and Waschewsky (1998)</td>
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<td>Régimbal and Mozurkewich (1997)</td>
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<td>(at 200 K)</td>
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<td>NH$_3$</td>
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<td>2000</td>
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<td>ROOH</td>
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<td>Lind and Kok (1994)</td>
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<td>Magi et al. (1997)</td>
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<td>$7.0 \times 10^3$</td>
<td>6425</td>
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<td>(at 260-270 K)</td>
<td>DeMore et al. (1997)</td>
</tr>
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<td>2000</td>
<td>estimated</td>
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<td>9001</td>
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<td>3072</td>
<td>Schweitzer et al. (2000)</td>
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<td>Huthwelker et al. (1995)</td>
<td>=HOBr</td>
<td>=HOBr</td>
<td>estimated</td>
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<tr>
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<td>estimated</td>
<td>0.1</td>
<td>(at RT)</td>
<td>Koch and Rossi (1998)</td>
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<td>Wilhelm et al. (1977)</td>
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<td>Hu et al. (1995)</td>
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<td>Vogt et al. (1996)</td>
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<td>(at RT)</td>
<td>Abbatt and Waschewsky (1998)</td>
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<tr>
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<td>Bartlett and Margerum (1999)</td>
<td>=Cl$_2$</td>
<td>=Cl$_2$</td>
<td>estimated</td>
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<tr>
<td>DMSO$_2$</td>
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<td>=HCHO</td>
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<td>2578</td>
<td>De Bruyn et al. (1994)</td>
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<td>0.076</td>
<td>1762</td>
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Table 6: Continued.

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<th>reference</th>
<th>$\alpha^0$</th>
<th>$-\Delta_{obs} H/R$ [K]</th>
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<td>0.5</td>
<td>2000</td>
<td>estimated by Vogt et al. (1999)</td>
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<td>=HOCl</td>
<td>Chatfield and Crutzen (1990)</td>
<td>=HOBr</td>
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<td>estimated by Vogt et al. (1999)</td>
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<td>estimated by Vogt et al. (1999)</td>
</tr>
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<td>2000</td>
<td>estimated by Vogt et al. (1999)</td>
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<td>—</td>
<td>0.01</td>
<td>2000</td>
<td>estimated by Vogt et al. (1999)</td>
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</table>

For ROOH the values of CH$_3$OOH have been assumed. The temperature dependence is for the Henry constants is $K_H = K_H^0 \times \exp(-\Delta_{soln} H R/(1/T - 1/T_0))$, $T_0 = 298$ K and for the accommodation coefficients $\frac{d \ln(\frac{1}{\alpha})}{dT} = -\frac{\Delta_{obs} H}{R}$. RT stands for “room temperature”.
References


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