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Supplement of

A mechanism for biologically induced iodine emissions from sea ice

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Table 1. Gas Phase Reactions and Rate Constants

#	Bimolecular Reactions	Rate Constants	References
1.	$O(^1D) + N_2 \rightarrow O + N_2$	$1.8 \times 10^{-11} e^{(110/T)}$	2
2.	$O(^1D) + O_2 \rightarrow O + O_2$	$3.2 \times 10^{-11} e^{(70/T)}$	2
3.	$O(^1D) + H_2O \rightarrow OH + OH$	2.2×10^{-10}	2
4.	$O(^1D) + CH_4 \rightarrow CH_3 + OH$ (0.75), $CH_3O + H$ (0.2), $HCHO + H_2$ (0.05)	1.5×10^{-10}	2
5.	$O(^1D) + H_2 \rightarrow OH + H$	1.1×10^{-10}	2
6.	$OH + CO \rightarrow H + CO_2$	$1.5 \times 10^{-13} \times (1 + 0.6 \times P_{atm})$	2
7.	$HO_2 + NO \rightarrow NO_2 + OH$	$3.5 \times 10^{-12} e^{(250/T)}$	2
8.	$O_3 + HO_2 \rightarrow OH + 2O_2$	$1.1 \times 10^{-14} e^{(-500/T)}$	2
9.	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$2.3 \times 10^{-13} e^{(600/T)}$	2
10.	$OH + H_2 \rightarrow H_2O + H$	$5.5 \times 10^{-12} e^{(-2000/T)}$	2
11.	$O_3 + OH \rightarrow HO_2 + O_2$	$1.6 \times 10^{-12} e^{(-940/T)}$	2
12.	$OH + HNO_3 \rightarrow H_2O + NO_3$	$k_0 = 7.2 \times 10^{-15} e^{(785/T)}$ $k_2 = 4.1 \times 10^{-16} e^{(1440/T)}$ $k_3 = 1.9 \times 10^{-33} e^{(725/T)}$ $k = k_0 + (k_3 \times [M]) / (1 + k_3 \times [M] / k_2)$	2
13.	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$2.9 \times 10^{-12} e^{(-160/T)}$	2
14.	$OH + HO_2NO_2 \rightarrow NO_2 + HO_2 + OH$	$1.3 \times 10^{-12} e^{(380/T)}$	2
15.	$OH + HO_2 \rightarrow H_2O + O_2$	$4.8 \times 10^{-11} e^{(250/T)}$	2
16.	$OH + HONO \rightarrow H_2O + NO_2$	$1.8 \times 10^{-11} e^{(390/T)}$	2
17.	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	2×10^{-14}	2,b
18.	$OH + CH_4 \rightarrow CH_3 + H_2O$	$2.45 \times 10^{-12} e^{(-1775/T)}$	2
19.	$O(^3P) + CH_3 \rightarrow CH_3O$	1.1×10^{-10}	2
20.	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	$3.8 \times 10^{-13} e^{(800/T)}$	2
21.	$CH_3OOH + OH \rightarrow CH_3(O)O + H_2O$	$0.7 \times 3.8 \times 10^{-12} e^{(200/T)}$	2
22.	$CH_3O + O_2 \rightarrow CH_2O + HO_2$	$3.9 \times 10^{-14} e^{(-900/T)}$	2
23.	$OH + HCHO \rightarrow H_2O + HCO$	$8.8 \times 10^{-12} e^{(25/T)}$	2
24.	$HCO + O_2 \rightarrow CO + HO_2$	$3.5 \times 10^{-12} e^{(140/T)}$	2
25.	$CH_3O_2 + CH_3O_2 \rightarrow 2CH_3O + O_2$ 29%	$0.29 \times 2.5 \times 10^{-13} e^{(190/T)}$	2
26.	$NO + CH_3O_2 \rightarrow NO_2 + CH_3O$	$3 \times 10^{-12} e^{(280/T)}$	2
27.	$NO + O_3 \rightarrow NO_2 + O_2$	$2 \times 10^{-12} e^{(-1400/T)}$	2
28.	$NO + NO_3 \rightarrow 2NO_2$	$1.5 \times 10^{-11} e^{(170/T)}$	2
29.	$NO_3 + HCHO \rightarrow$ Products	5.8×10^{-16}	2,b
30.	$HO_2 + SO_2 \rightarrow$ Products	1×10^{-18}	2,b
31.	$N_2O_5 + H_2O \rightarrow 2HNO_3$	2.5×10^{-22}	2,b
32.	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2 \times 10^{-13} e^{(-2450/T)}$	2
33.	$OH + O(^3P) \rightarrow H + O_2$	$2.2 \times 10^{-11} e^{(120/T)}$	2
34.	$O(^3P) + HO_2 \rightarrow OH + O_2$	$3 \times 10^{-11} e^{(200/T)}$	2

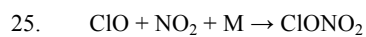
35.	$\text{H}_2\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{HO}_2$	$1.4 \times 10^{-12} e^{(-2000/T)}$	2
36.	$\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}(^3\text{P})$	$4.2 \times 10^{-12} e^{(-240/T)}$	2
37.	$\text{O}_3 + \text{Alkenes} \rightarrow \text{Products}$	$1.2 \times 10^{-14} e^{(-2630/T)}$	2,b
38.	$\text{NO}_3 + \text{CO} \rightarrow \text{Products}$	4×10^{-19}	2,b
39.	$\text{OH} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_2\text{OOH} + \text{H}_2\text{O} \rightarrow \text{CH}_2\text{O} + \text{OH} + \text{H}_2\text{O}$	$0.3 \times 3.8 \times 10^{-12} e^{(200/T)}$	2
40.	$\text{O}(^3\text{P}) + \text{HCHO} \rightarrow \text{OH} + \text{HCO}$	$3.4 \times 10^{-11} e^{(-1600/T)}$	2
41.	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HO}_2\text{CH}_2\text{O}$	$6.7 \times 10^{-15} e^{(600/T)}$	2
42.	$\text{H} + \text{O}_3 \rightarrow \text{OH} + \text{O}_2$	$1.4 \times 10^{-10} e^{(-470/T)}$	2
43.	$\text{HO}_2 + \text{H} \rightarrow 2\text{OH}$	$0.9 \times 8.1 \times 10^{-11}$	2
44.	$\text{O}(^3\text{P}) + \text{HO}_2\text{NO}_2 \rightarrow \text{Products}$	$7.8 \times 10^{-11} e^{(-3400/T)}$	2
45.	$\text{O}(^1\text{D}) + \text{O}_3 \rightarrow 2\text{O}_2$	1.2×10^{-10}	2
46.	$\text{O}(^1\text{D}) + \text{O}_3 \rightarrow \text{O}_2 + 2\text{O}$	1.2×10^{-10}	2
47.	$\text{CH}_3\text{O}_2 + \text{SO}_2 \rightarrow \text{Products}$	5×10^{-17}	1,b
48.	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{OH} + \text{NO}_2 + \text{O}_2$	3.5×10^{-12}	2
49.	$\text{CH}_3 + \text{O}_3 \rightarrow \text{Products}$	$5.4 \times 10^{-12} e^{(-220/T)}$	2
50.	$\text{SO}_2 + \text{O}_3 \rightarrow \text{SO}_3 + \text{O}_2$	$3 \times 10^{-12} e^{(-7000/T)}$	2,b
51.	$\text{NO}_3 + \text{OH} \rightarrow \text{NO}_2 + \text{HO}_2$	2.2×10^{-11}	2
52.	$\text{O}_3 + \text{O}(^3\text{P}) \rightarrow 2\text{O}_2$	$8 \times 10^{-12} e^{(-2060/T)}$	2
53.	$\text{O}_3 + \text{HONO} \rightarrow \text{O}_2 + \text{HNO}_3$	5×10^{-19}	2,b
54.	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{Products}$	3×10^{-17}	2,b
55.	$\text{NO}_3 + \text{Alkenes} \rightarrow \text{HOCH}_2\text{CH}_2 + \text{NO}_2$	3×10^{-14}	1
56.	$\text{SO}_2 + \text{NO}_2 \rightarrow \text{Products}$	2×10^{-26}	1,b
57.	$\text{NO}_3 + \text{Alkanes} \rightarrow \text{C}_2\text{H}_5 + \text{HNO}_3$	3.6×10^{-17}	1
58.	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{CH}_3\text{OH} + \text{O}_2$	$0.71 \times 2.5 \times 10^{-13} e^{(190/T)}$	2
59.	$\text{NO}_2 + \text{NO}_3 \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2$	$4.5 \times 10^{-14} e^{(-1260/T)}$	2
60.	$\text{OH} + \text{Alkanes} \rightarrow \text{C}_2\text{H}_5 + \text{H}_2\text{O}$	$1.1 \times 10^{-11} e^{(-1100/T)}$	1
61.	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}$	$2.6 \times 10^{-12} e^{(365/T)}$	2
62.	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CH}_3\text{CO} (\rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2)$	$1.4 \times 10^{-12} e^{(-1900/T)}$	2
63.	$\text{CH}_3\text{CHO} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{CH}_3\text{CO} (\rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2)$	$1.8 \times 10^{-11} e^{(-1100/T)}$	2
64.	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CO} (\rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2)$	$5.6 \times 10^{-12} e^{(270/T)}$	2
65.	$\text{O}(^3\text{P}) + \text{H}_2 \rightarrow \text{OH} + \text{H}$	4.11×10^{-18}	1
66.	$\text{NO} + \text{CH}_3\text{C}(\text{O})\text{O}_2 \rightarrow \text{NO}_2 + \text{CH}_3 + \text{CO}_2$	$5.3 \times 10^{-12} e^{(360/T)}$	2
67.	$\text{OH} + \text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_4\text{OOH} + \text{H}_2\text{O}$	3.64×10^{-12}	1
68.	$\text{OH} + \text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	5.95×10^{-12}	1
69.	$\text{NO}_2 + \text{O}(^3\text{P}) \rightarrow \text{NO} + \text{O}_2$	$6.5 \times 10^{-12} e^{(120/T)}$	2
70.	$\text{NO}_3 + \text{O}(^3\text{P}) \rightarrow \text{NO}_2 + \text{O}_2$	1×10^{-11}	2
71.	$\text{HNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{NO}_3 + \text{OH}$	3×10^{-17}	2,b
71.	$\text{C}_2\text{H}_5\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$6.3 \times 10^{-14} e^{(-550/T)}$	2
73.	$\text{HO}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{CH}_2\text{O}$	$2.4 \times 10^{12} e^{(-7000/T)}$	1
74.	$\text{HO}_2\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{HCOOH} + \text{O}_2 + \text{H}_2\text{O}$	$5.6 \times 10^{-15} e^{(2300/T)}$	1
	Halogen chemistry		
75.	$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	$2 \times 10^{-11} e^{(-890/T)}$	2
76.	$\text{I} + \text{HO}_2 \rightarrow \text{HI} + \text{O}_2$	$1.5 \times 10^{-11} e^{(-1190/T)}$	2
77.	$\text{IO} + \text{NO} \rightarrow \text{I} + \text{NO}_2$	$7.3 \times 10^{-12} e^{(330/T)}$	2
78.	$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	5.8×10^{-11}	2

79.	$\text{IO} + \text{IO} \rightarrow \text{OIO} + \text{I} / \text{I}_2\text{O}_2$	8.6×10^{-11}	3
80.	$\text{IO} + \text{OIO} (+\text{M}) \rightarrow \text{I}_2\text{O}_3$	1.5×10^{-11}	3
81.	$\text{IONO}_2 \rightarrow \text{IO} + \text{NO}_2$	$2.07 \times 10^{15} e^{(-11859/T)}$	2
82.	$\text{OH} + \text{HI} \rightarrow \text{I} + \text{H}_2\text{O}$	3×10^{-11}	2
83.	$\text{HOI} + \text{OH} \rightarrow \text{IO} + \text{H}_2\text{O}$	2×10^{-13}	2
84.	$\text{IO} + \text{DMS} \rightarrow \text{Products}$	1.2×10^{-14}	2
85.	$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	$(2.4 / 0.005) \times 2.07 \times 10^{15} e^{(-11859/T)}$	2
86.	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7 \times 10^{-11} e^{(-800/T)}$	2
87.	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	1.1×10^{-11}	2
88.	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$1.5 \times 10^{-11} e^{(-600/T)}$	2
89.	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{HCO}$	$7.7 \times 10^{-13} e^{(-580/T)}$	2
90.	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{CO}$	$1.8 \times 10^{-12} e^{(-460/T)}$	2
91.	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$3.4 \times 10^{-12} e^{(540/T)}$	2
92.	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.8 \times 10^{-12} e^{(260/T)}$	2
93.	$\text{BrO} + \text{CH}_3\text{SCH}_3 \rightarrow \text{CH}_3\text{SOCH}_3 + \text{Br}$	$1.5 \times 10^{-14} e^{(850/T)}$	2
94.	$\text{BrO} + \text{BrO} \rightarrow 2\text{Br} + \text{O}_2$	$2.4 \times 10^{-12} e^{(40/T)}$	2
95.	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.8 \times 10^{-14} e^{(860/T)}$	2
96.	$\text{BrONO}_2 \rightarrow \text{BrO} + \text{NO}_2$	$2.8 \times 10^{13} e^{-(12360/T)}$	4
97.	$\text{BrO} + \text{IO} \rightarrow \text{Br} + \text{I} + \text{O}_2 / \text{Br} + \text{OIO}$	$1.5 \times 10^{-12} e^{(510/T)}$	2
98.	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$	$1.1 \times 10^{-11} e^{(-1400/T)}$	2
99.	$\text{HCl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	$2.6 \times 10^{-12} e^{(-350/T)}$	2
100.	$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	$2.9 \times 10^{-11} e^{(-260/T)}$	2
101.	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	$5.0 \times 10^{-12} e^{(700/T)}$	2
102.	$\text{ClO} + \text{NO} \rightarrow \text{Cl} + \text{NO}_2$	$6.4 \times 10^{-12} e^{(290/T)}$	2
103.	$\text{ClO} + \text{IO} \rightarrow 0.2 (\text{I} + \text{Cl} + \text{O}_2)$	$1.3 \times 10^{-12} e^{(280/T)}$	2
104.	$\text{Cl} + \text{Alkanes} \rightarrow \text{HCl} + \text{CH}_3\text{OO}$	$5.7 \times 10^{-11} e^{(-90/T)}$	2,1
105.	$\text{Cl} + \text{Alkenes} \rightarrow \text{HCl} + \text{CH}_3\text{OO}$	1.0×10^{-10}	2,1
106.	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{HO}_2 + \text{CO}$	$7.3 \times 10^{-11} e^{(-30/T)}$	2
107.	$\text{ClO} + \text{CH}_3\text{OO} \rightarrow \text{Cl} + \text{HCHO} + \text{HO}_2$	$2.2 \times 10^{-12} e^{(-115/T)}$	2
108.	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$	3.5×10^{-13}	2
109.	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	50	2
110.	$\text{ClONO}_2 \rightarrow \text{ClO} + \text{NO}_2$	0.0022	2
111.	$\text{Cl} + \text{ClONO}_2 \rightarrow \text{Cl}_2 + \text{NO}_3$	$9.6 \times 10^{-12} e^{(140/T)}$	2
112.	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	$4.1 \times 10^{-13} e^{(-980/T)}$	2
113.	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$1.2 \times 10^{-10} e^{(-260/T)}$	2,1
114.	$\text{BrCl} + \text{Br} \rightarrow \text{Br}_2 + \text{Cl}$	3.3×10^{-15}	2,1
115.	$\text{Cl}_2 + \text{Br} \rightarrow \text{BrCl} + \text{Cl}$	1.1×10^{-15}	2,1
116.	$\text{BrCl} + \text{Cl} \rightarrow \text{Cl}_2 + \text{Br}$	1.5×10^{-11}	2,1
117.	$\text{ClO} + \text{BrO} \rightarrow \text{Br} + \text{OClO}$	$6.0 \times 10^{-12} e^{(550/T)}$	2,1
118.	$\text{ClO} + \text{BrO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$5.6 \times 10^{-12} e^{(260/T)}$	2,1
119.	$\text{ClO} + \text{BrO} \rightarrow \text{BrCl} + \text{O}_2$	$1.1 \times 10^{-12} e^{(290/T)}$	2,1

Recombination Reactions

1.	$\text{O}(\text{D}) + \text{N}_2 (+\text{M}) \rightarrow \text{N}_2\text{O} (+\text{M})$	$[\text{M}] \times 3.5 \times 10^{-37} \times (\text{T} / 300)^{-0.6}$	2
2.	$\text{HO}_2 + \text{HO}_2 (+\text{M}) \rightarrow \text{H}_2\text{O}_2 (+\text{M})$	$[\text{M}] \times 1.7 \times 10^{-33} e^{(1000/T)}$	2
3.	$\text{H} + \text{O}_2 (+\text{M}) \rightarrow \text{HO}_2 (+\text{M})$	$k_0 = 5.7 \times 10^{-32} \times (\text{T} / 300)^{-1.6}$	2

4.	$O_2 + O(^3P) \rightarrow O_3$	$k_{\infty} = 7.5 \times 10^{-11}$ $[M] \times 6 \times 10^{-34} \times (T / 300)^{-2.3}$	2
5.	$NO_2 + OH \rightarrow HNO_3$	$k_0 = 2.5 \times 10^{-30} \times (T / 300)^{-4.4}$ $k_{\infty} = 1.6 \times 10^{-11} \times (T / 300)^{-1.7}$	2
6.	$NO + OH (+ M) \rightarrow HONO (+ M)$	$k_0 = 7 \times 10^{-31} \times (T / 300)^{-2.6}$ $k_{\infty} = 1.5 \times 10^{-11} \times (T / 300)^{-0.5}$	2
7.	$HO_2 + NO_2 (+ M) \rightarrow HO_2NO_2 (+ M)$	$k_0 = 1.8 \times 10^{-31} \times (T / 300)^{-3.2}$ $k_{\infty} = 4.7 \times 10^{-12} \times (T / 300)^{-1.4}$	2
8.	$HO_2NO_2 \rightarrow HO_2 + NO_2$	$k_R = k_F / k_{EQ}$ $k_R = k_F / (2.1 \times 10^{-27} e^{(10900/T)})$	2
9.	$O_2 + CH_3 (+ M) \rightarrow CH_3O_2 (+ M)$	$k_0 = 4.5 \times 10^{-31} \times (T / 300)^{-3}$ $k_{\infty} = 1.8 \times 10^{-12} \times (T / 300)^{-1.7}$	2
10.	$NO_2 + NO_3 (+ M) \rightarrow N_2O_5 (+ M)$	$k_0 = 2.2 \times 10^{-30} \times (T / 300)^{-3.9}$ $k_{\infty} = 1.5 \times 10^{-12} \times (T / 300)^{-0.7}$	2
11.	$N_2O_5 (+ N_2) \rightarrow NO_2 + NO_3 (+ N_2)$	$k_R = k_F / k_{EQ}$ $k_R = k_F / (2.7 \times 10^{-27} e^{(11000/T)})$	2
12.	$OH + OH (+ M) \rightarrow H_2O_2 (+ M)$	$k_0 = 6.2 \times 10^{-31} \times (T / 300)^{-1}$ $k_{\infty} = 2.6 \times 10^{-11}$	2
13.	$NO + O(^3P) (+ M) \rightarrow NO_2 (+ M)$	$k_0 = 9 \times 10^{-32} \times (T / 300)^{-1.5}$ $k_{\infty} = 3 \times 10^{-11}$	2
14.	$NO_2 + O(^3P) (+ M) \rightarrow NO_3 (+ M)$	$k_0 = 9 \times 10^{-32} \times (T / 300)^{-2}$ $k_{\infty} = 2.2 \times 10^{-11}$	2
15.	$SO_2 + OH (+ M) \rightarrow HOSO_2 (+ M)$	$k_0 = 3 \times 10^{-31} \times (T / 300)^{-3.3}$ $k_{\infty} = 1.5 \times 10^{-12}$	2
16.	$CH_3C(O)O_2 + NO_2 (+ M) \rightarrow PAN (+ M)$	$k_0 = 9.7 \times 10^{-29} \times (T / 300)^{-5.6}$ $k_{\infty} = 9.3 \times 10^{-12} \times (T / 300)^{-1.5}$	2
17.	$PAN (+ M) \rightarrow CH_3C(O)O_2 + NO_2 (+ M)$	$k_R = k_F / k_{EQ}$ $k_R = k_F / (9 \times 10^{-29} e^{(14000/T)})$	2
18.	$OH + Alkenes (+ M) \rightarrow HOCH_2CH_2 (+ M)$	$k_0 = 1.5 \times 10^{-28} \times (T / 300)^{-0.8}$ $k_{\infty} = 8.8 \times 10^{-12}$	2,1
19.	$C_2H_5 + O_2 (+ M) \rightarrow C_2H_5O_2 (+ M)$	$k_0 = 1.5 \times 10^{-28} \times (T / 300)^{-3.8}$ $k_{\infty} = 8 \times 10^{-12}$	2
20.	$NO_2 + CH_3O_2 (+ M) \rightarrow CH_3O_2NO_2 (+ M)$	$k_0 = 1.5 \times 10^{-30} \times (T / 300)^{-4}$ $k_{\infty} = 6.5 \times 10^{-12} \times (T / 300)^{-2}$	2
21.	$CH_3O_2NO_2 \rightarrow CH_3O_2 + NO_2$	$k_R = k_F / k_{EQ}$ $k_R = k_F / (1.3 \times 10^{-28} e^{(11200/T)})$	2
22.	$I + NO_2 (+ M) \rightarrow INO_2 (+ M)$	$k_0 = 3 \times 10^{-31} \times (T / 300)^{-1}$ $k_{\infty} = 6.6 \times 10^{-11}$ $F_c = e^{(-T/650)} + e^{(-2600/T)}$	2
23.	$IO + NO_2 (+ M) \rightarrow IONO_2 (+ M)$	$k_0 = 7.7 \times 10^{-31} \times (T / 300)^{-5}$ $k_{\infty} = 1.6 \times 10^{-11}$ $F_c = 0.4$	2
24.	$Br + NO_2 + M \rightarrow BrNO_2$	$k_0 = 4.2 \times 10^{-31} \times (T / 300)^{-2.4}$ $k_{\infty} = 2.7 \times 10^{-11} \times (T / 300)^{-0}$	2
25.	$BrO + NO_2 + M \rightarrow BrONO_2$	$k_0 = 5.2 \times 10^{-31} \times (T / 300)^{-3.2}$	2



$$k = 6.9 \times 10^{-12} \times (T / 300)^{-2.9}$$

$$k_0 = 1.62 \times 10^{-31} \times (T / 300)^{-3.4}$$

$$k_\infty = 1.5 \times 10^{-11}$$

2

	Photochemical Reactions	References
J1.	$\text{O}_3 + h\nu \rightarrow \text{O}_2 + \text{O}(^1\text{D})$	2,1,c
J2.	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2\text{OH}$	2,1,c
J3.	$\text{HNO}_3 + h\nu \rightarrow \text{OH} + \text{NO}_2$	2,1,c
J4.	$\text{HO}_2\text{NO}_2 + h\nu \rightarrow \text{OH} + \text{NO}_3$	2,1,c
J5.	$\text{HONO} + h\nu \rightarrow \text{OH} + \text{NO}$	2,1,c
J6.	$\text{CH}_3\text{OOH} + h\nu \rightarrow \text{CH}_3\text{O} + \text{OH}$	2,1,c
J7.	$\text{CH}_2\text{O} + h\nu \rightarrow \text{HCO} + \text{H}$	2,1,c
J8.	$\text{CH}_2\text{O} + h\nu \rightarrow \text{CO} + \text{H}_2$	2,1,c
J9.	$\text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O}$	2,1,c
J10.	$\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{O}$	2,1,c
J11.	$\text{N}_2\text{O}_5 + h\nu \rightarrow \text{NO}_2 + \text{NO}_3$	2,1,c
J12.	$\text{C}_2\text{H}_5\text{O}_2\text{H} + h\nu \rightarrow \text{OH} + \text{C}_2\text{H}_5\text{O}$	2,1,c
J13.	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_3 + \text{HCO}$	2,1,c
J15.	$\text{PAN} (\text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2) + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO}_2$	2,1,c
J16.	$\text{NO}_3 + h\nu \rightarrow \text{NO} + \text{O}_2$	2,1,c
J17.	$\text{CH}_3\text{I} + h\nu \rightarrow \text{CH}_3 + \text{I}$	2,1,c
J18.	$\text{CH}_2\text{I}_2 + h\nu \rightarrow \text{CH}_2\text{I} + \text{I} \rightarrow \text{CH}_2 + 2\text{I}$	2,1,c
J19.	$\text{CH}_2\text{IBr} + h\nu \rightarrow \text{CH}_2\text{Br} + \text{I}$	2,1,c
J20.	$\text{I}_2 + h\nu \rightarrow 2\text{I}$	2,1,c
J21.	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2 / \text{IO} + \text{NO}$	2,1,c
J22.	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}$	2,1,c
J23.	$\text{OIO} + h\nu \rightarrow \text{I} + \text{O}_2$	2,1,c
J24.	$\text{IONO}_2 + h\nu \rightarrow \text{I} + \text{NO}_3$	2,1,c
J25.	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	2,1,c
J26.	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}$	2,1,c
J27.	$\text{Br}_2 + h\nu \rightarrow 2\text{Br}$	2,1,c
J28.	$\text{IBr} + h\nu \rightarrow \text{Br} + \text{I}$	2,1,c
J29.	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	2,1,c
J30.	$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$	2,1,c
J31.	$\text{BrONO}_2 + h\nu \rightarrow 0.7 (\text{BrO} + \text{NO}_2) / 0.3 (\text{Br} + \text{NO}_3)$	2,1,c
J32.	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	2,1,c
J33.	$\text{Cl}_2 + h\nu \rightarrow 2\text{Cl}$	2,1,c
J34.	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	2,1,c
J35.	$\text{ClO} + h\nu \rightarrow \text{Cl} + \text{O}$	2,1,c
J36.	$\text{HOCl} + h\nu \rightarrow \text{Cl} + \text{OH}$	2,1,c
J37.	$\text{ClONO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$	2,1,c
J38.	$\text{ClONO}_2 + h\nu \rightarrow 0.9 (\text{Cl} + \text{NO}_3) / 0.1 (\text{ClO} + \text{NO}_2)$	2,1,c

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Species	Deposition velocities, cm s ⁻¹	References
HOI	1.0	5
HOBr	1.0	d
HOCl	1.0	d
HBr	2.0	d
HCl	2.0	d
HI	1.0	5
BrONO ₂	1.0	d
IONO ₂	1.0	5
ClONO ₂	1.0	d
INO ₂	1.0	d

^aUnits: unimolecular reactions, s⁻¹; photolysis rate constants, s⁻¹; bimolecular reactions, cm³ molecule⁻¹ s⁻¹; termolecular reactions, cm⁶ molecule⁻² s⁻¹, calculated using the formalism of *Sander et al. (2006)*, where $k = ((k_0 [M]/(1 + k_0[M]/k_\infty)) \times F_c^n)$, $F_c = 0.6$ (unless otherwise noted) and $n = (1 + (\log_{10}(k_0[M]/k_\infty))^2)^{-1}$.

60

^bset as upper limit.

^cabsorption cross-sections taken from *Atkinson et al., 2000*.

65

^ddeposition velocities estimated.

Table 2. QLL Reactions and Rate Constants

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#	Reactions	Rate Constants	References
1.	HOI + I ⁻ + H ⁺ → I ₂ + H ₂ O	4.4 x 10 ¹² M ⁻² s ⁻¹ /(volumetric) ²	6
2.	I ₂ + H ₂ O → HOI + I ⁻ + H ⁺	0 s ⁻¹	
3.	HOI + Br ⁻ + H ⁺ → IBr + H ₂ O	3.3 x 10 ¹² M ⁻² s ⁻¹ /(volumetric) ²	7
4.	IBr + H ₂ O → HOI + Br ⁻ + H ⁺	8.0 x 10 ⁵ s ⁻¹	7
5.	HOI + Cl ⁻ + H ⁺ → ICl + H ₂ O	2.9 x 10 ¹⁰ M ⁻² s ⁻¹ /(volumetric) ²	8
6.	ICl + H ₂ O → HOI + Cl ⁻ + H ⁺	2.4 x 10 ⁶ s ⁻¹	8
7.	HOBr + Br ⁻ + H ⁺ → Br ₂ + H ₂ O	1.6 x 10 ¹⁰ M ⁻² s ⁻¹ /(volumetric) ²	9
8.	Br ₂ + H ₂ O → HOBr + Br ⁻ + H ⁺	9.7 x 10 ¹ s ⁻¹	9
9.	HOBr + Cl ⁻ + H ⁺ → BrCl + H ₂ O	5.6 x 10 ⁹ M ⁻² s ⁻¹ /(volumetric) ²	10
10.	BrCl + H ₂ O → HOBr + Cl ⁻ + H ⁺	1.0 x 10 ⁵ s ⁻¹	10
11.	BrCl + Br ⁻ → Br ₂ Cl ⁻	5.0 x 10 ⁹ M ⁻¹ s ⁻¹ /(volumetric)	10
12.	Br ₂ Cl ⁻ → BrCl + Br ⁻	2.8 x 10 ⁵ s ⁻¹	10
13.	Br ₂ Cl ⁻ → Br ₂ + Cl ⁻	3.8 x 10 ⁹ s ⁻¹	10
14.	Br ₂ + Cl ⁻ → Br ₂ Cl ⁻	5.0 x 10 ⁹ M ⁻¹ s ⁻¹ /(volumetric)	10
15.	BrCl + Cl ⁻ → BrCl ₂ ⁻	5.0 x 10 ⁹ M ⁻¹ s ⁻¹ /(volumetric)	11

16.	$\text{BrCl}_2^- \rightarrow \text{BrCl} + \text{Cl}^-$	$1.3 \times 10^9 \text{ s}^{-1}$	11
17.	$\text{HOBr} + \text{I}^- \rightarrow \text{IBr} + \text{OH}^-$	$5.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}/(\text{volumetric})$	12
18.	$\text{HOCl} + \text{Cl}^- + \text{H}^+ \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	$2.2 \times 10^4 \text{ e}^{(-3508/T)} \text{ M}^{-2} \text{ s}^{-1}/(\text{volumetric})^2$	13
19.	$\text{Cl}_2 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{Cl}^- + \text{H}^+$	$2.2 \times 10^1 \text{ e}^{(-8012/T)} \text{ s}^{-1}$	13
20.	$\text{HOCl} + \text{Br}^- + \text{H}^+ \rightarrow \text{BrCl} + \text{H}_2\text{O}$	$3.5 \times 10^{11} \text{ M}^{-2} \text{ s}^{-1}/(\text{volumetric})^2$	14
21.	$\text{BrCl} + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{Br}^- + \text{H}^+$	0 s^{-1}	
22.	$\text{HOCl} + \text{I}^- + \text{H}^+ \rightarrow \text{ICl} + \text{H}_2\text{O}$	$3.9 \times 10^{-14} \text{ e}^{(-900/T)} \text{ M}^{-2} \text{ s}^{-1}/(\text{volumetric})^2$	15
23.	$\text{ICl} + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{I}^- + \text{H}^+$	0 s^{-1}	

Table 3. Henry Constants

Species	Henry Constants	References
IO	$4.5 \times 10^2 \text{ e}^{(5862(1/T - 1/T_0))} \text{ M atm}^{-1}$	16
HOI	$4.5 \times 10^2 \text{ e}^{(5862(1/T - 1/T_0))} \text{ M atm}^{-1}$	16,17
I ₂	$3.0 \times 10^0 \text{ e}^{(4431(1/T - 1/T_0))} \text{ M atm}^{-1}$	18
ICl	$1.1 \times 10^2 \text{ e}^{(5600(1/T - 1/T_0))} \text{ M atm}^{-1}$	19
IBr	$2.4 \times 10^1 \text{ e}^{(5600(1/T - 1/T_0))} \text{ M atm}^{-1}$	20
HOBr	$9.3 \times 10^1 \text{ e}^{(5862(1/T - 1/T_0))} \text{ M atm}^{-1}$	16,20
Br ₂	$7.6 \times 10^{-1} \text{ e}^{(4094(1/T - 1/T_0))} \text{ M atm}^{-1}$	21
BrCl	$9.4 \times 10^{-1} \text{ e}^{(5600(1/T - 1/T_0))} \text{ M atm}^{-1}$	17
HOCl	$6.7 \times 10^2 \text{ e}^{(5862(1/T - 1/T_0))} \text{ M atm}^{-1}$	17
Cl ₂	$9.1 \times 10^{-2} \text{ e}^{(2500(1/T - 1/T_0))} \text{ M atm}^{-1}$	22

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