Supplementary Online Material

Multiphase modeling of nitrate photochemistry in the quasi-liquid layer (QLL): Implications for NO_x release from the Arctic and coastal Antarctic snowpack

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This PDF file includes:

Supporting online text

Table 1

References

Radiation and gas phase scheme

Photolysis rates are calculated off-line from reported absorption cross-sections and quantum yields using a 2-stream radiative transfer code,[1] where the irradiance reaching the surface is computed after photon attenuation through fifty 1 km layers in the atmosphere.

Some species in the model are constrained to their typical values measured during the Chemistry of the Antarctic Boundary Layer and Interface with Snow (CHABLIS) measurement field campaign that took place at Halley Bay in coastal Antarctica[2,3] with diurnal mixing ratio profiles peaking at [CO] = 35 ppb; [DMS] = 80 ppt; [SO_2] = 15 ppt; [CH_4] = 1750 ppb; [CH_3CHO] = 150 ppt; [HCHO] = 150 ppt; [isoprene] = 60 ppt; [propane] = 25 ppt; [propene] = 15 ppt. During the model simulations all other species are allowed to vary. The model is solved using a variable step-size fourth-order Runge-Kutta integrator.

The dry deposition of a species i is computed as $V_iC_i(t)/H$, where C is the concentration of a gaseous species at a given time and V_i is the deposition velocity of species over a fixed boundary layer over time with a depth H of 100 m.

Table 1. Gas Phase Reactions and Rate Constants

#	Bimolecular Reactions	Rate Constants	References
1.	$O(^1D) + N_2 \rightarrow O + N_2$	$1.8 \times 10^{-11} e^{(110 / T)}$	5
2.	$O(^1D) + O_2 \rightarrow O + O_2$	$3.2 \times 10^{-11} e^{(70 / T)}$	5
3.	$O(^1D) + H_2O \rightarrow OH + OH$	2.2×10^{-10}	5
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}	5
5.	$O(^1D) + H_2 \rightarrow OH + H$	1.1×10^{-10}	5
6.	$OH + CO \rightarrow H + CO_2$	$1.5 \times 10^{-13} \times (1 + 0.6 \times P_{atm})$	5
7.	$HO_2 + NO \rightarrow NO_2 + OH$	$3.5 \times 10^{-12} e^{(250 / T)}$	5
8.	$O_3 + HO_2 \rightarrow OH + 2O_2$	$1.1 \times 10^{-14} e^{(-500 / T)}$	5
9.	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$2.3 \times 10^{-13} e^{(600 / T)}$	5
10.	$OH + H_2 \rightarrow H_2O + H$	$5.5 \times 10^{-12} e^{(-2000 / T)}$	5
11.	$O_3 + OH \rightarrow HO_2 + O_2$	$1.6 \times 10^{-12} e^{(-940 / T)}$	5
12.	$OH + HNO_3 \rightarrow H_2O + NO_3$	$k_0 = 7.2 \times 10^{-15} e^{(785 / T)}$ $k_2 = 4.1 \times 10^{-16} e^{(1440 / T)}$ $k_3 = 1.9 \times 10^{-33} e^{(725 / T)}$ $k = k_0 + (k_3 \times [M] / (1 + k_3 \times [M] / k_2))$	5
13.	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$2.9 \times 10^{-12} e^{(-160 / T)}$	5
14.	$OH + HO_2NO_2 \rightarrow NO_2 + HO_2 + OH$	$1.3 \times 10^{-12} e^{(380 / T)}$	5
15.	$OH + HO_2 \rightarrow H_2O + O_2$	$4.8 \times 10^{-11} e^{(250 / T)}$	5
16.	$OH + HONO \rightarrow H_2O + NO_2$	$1.8 \times 10^{-11} e^{(390 / T)}$	5
17.	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	2×10^{-14}	5,b
18.	$OH + CH_4 \rightarrow CH_3 + H_2O$	$2.45 \times 10^{-12} e^{(-1775 / T)}$	5
19.	$O(^3P) + CH_3 \rightarrow CH_3O$	1.1×10^{-10}	5
20.	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	$3.8 \times 10^{-13} e^{(800 / T)}$	5
21.	$CH_3OOH + OH \rightarrow CH_3(O)O + H_2O$	$0.7 \times 3.8 \times 10^{-12} e^{(200 / T)}$	5
22.	$CH_3O + O_2 \rightarrow CH_2O + HO_2$	$3.9 \times 10^{-14} e^{(-900 / T)}$	5
23.	$OH + HCHO \rightarrow H_2O + HCO$	$8.8 \times 10^{-12} e^{(25 / T)}$	5
24.	$HCO + O_2 \rightarrow CO + HO_2$	$3.5 \times 10^{-12} e^{(140 / T)}$	5
25.	$CH_3O_2 + CH_3O_2 \rightarrow 2CH_3O + O_2$ 29%	$0.29 \times 2.5 \times 10^{-13} e^{(190 / T)}$	5
26.	$NO + CH_3O_2 \rightarrow NO_2 + CH_3O$	$3 \times 10^{-12} e^{(280 / T)}$	5
27.	$NO + O_3 \rightarrow NO_2 + O_2$	$2 \times 10^{-12} e^{(-1400 / T)}$	5
28.	$NO + NO_3 \rightarrow 2NO_2$	$1.5 \times 10^{-11} e^{(170 / T)}$	5
29.	$NO_3 + HCHO \rightarrow$ Products	5.8×10^{-16}	5,b
30.	$HO_2 + SO_2 \rightarrow$ Products	1×10^{-18}	5,b
31.	$N_2O_5 + H_2O \rightarrow 2HNO_3$	2.5×10^{-22}	5,b
32.	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2 \times 10^{-13} e^{(-2450 / T)}$	5
33.	$OH + O(^3P) \rightarrow H + O_2$	$2.2 \times 10^{-11} e^{(120 / T)}$	5
34.	$O(^3P) + HO_2 \rightarrow OH + O_2$	$3 \times 10^{-11} e^{(200 / T)}$	5
35.	$H_2O_2 + O(^3P) \rightarrow OH + HO_2$	$1.4 \times 10^{-12} e^{(-2000 / T)}$	5
36.	$OH + OH \rightarrow H_2O + O(^3P)$	$4.2 \times 10^{-12} e^{(-240 / T)}$	5
37.	$O_3 + Alkenes \rightarrow$ Products	$1.2 \times 10^{-14} e^{(-2630 / T)}$	5,b

38.	$NO_3 + CO \rightarrow$ Products	4×10^{-19}	5,b
39.	$OH + CH_3OOH \rightarrow CH_2OOH + H_2O \rightarrow CH_2O + OH + H_2O$	$0.3 \times 3.8 \times 10^{-12} e^{(200 / T)}$	5
40.	$O(^3P) + HCHO \rightarrow OH + HCO$	$3.4 \times 10^{-11} e^{(-1600 / T)}$	5
41.	$HCHO + HO_2 \rightarrow HO_2CH_2O$	$6.7 \times 10^{-15} e^{(600 / T)}$	5
42.	$H + O_3 \rightarrow OH + O_2$	$1.4 \times 10^{-10} e^{(-470 / T)}$	5
43.	$HO_2 + H \rightarrow 2OH$	$0.9 \times 8.1 \times 10^{-11}$	5
44.	$O(^3P) + HO_2NO_2 \rightarrow$ Products	$7.8 \times 10^{-11} e^{(-3400 / T)}$	5
45.	$O(^1D) + O_3 \rightarrow 2O_2$	1.2×10^{-10}	5
46.	$O(^1D) + O_3 \rightarrow O_2 + 2O$	1.2×10^{-10}	5
47.	$CH_3O_2 + SO_2 \rightarrow$ Products	5×10^{-17}	4,b
48.	$NO_3 + HO_2 \rightarrow OH + NO_2 + O_2$	3.5×10^{-12}	5
49.	$CH_3 + O_3 \rightarrow$ Products	$5.4 \times 10^{-12} e^{(-220 / T)}$	5
50.	$SO_2 + O_3 \rightarrow SO_3 + O_2$	$3 \times 10^{-12} e^{(-7000 / T)}$	5,b
51.	$NO_3 + OH \rightarrow NO_2 + HO_2$	2.2×10^{-11}	5
52.	$O_3 + O(^3P) \rightarrow 2O_2$	$8 \times 10^{-12} e^{(-2060 / T)}$	5
53.	$O_3 + HONO \rightarrow O_2 + HNO_3$	5×10^{-19}	5,b
54.	$CH_3O_2 + O_3 \rightarrow$ Products	3×10^{-17}	5,b
55.	$NO_3 + Alkenes \rightarrow HOCH_2CH_2 + NO_2$	3×10^{-14}	4
56.	$SO_2 + NO_2 \rightarrow$ Products	2×10^{-26}	4,b
57.	$NO_3 + Alkanes \rightarrow C_2H_5 + HNO_3$	3.6×10^{-17}	4
58.	$CH_3O_2 + CH_3O_2 \rightarrow CH_2O + CH_3OH + O_2$	$0.71 \times 2.5 \times 10^{-13} e^{(190 / T)}$	5
59.	$NO_2 + NO_3 \rightarrow NO + NO_2 + O_2$	$4.5 \times 10^{-14} e^{(-1260 / T)}$	5
60.	$OH + Alkanes \rightarrow C_2H_5 + H_2O$	$1.1 \times 10^{-11} e^{(-1100 / T)}$	4
61.	$C_2H_5O_2 + NO \rightarrow NO_2 + C_2H_5O$	$2.6 \times 10^{-12} e^{(365 / T)}$	5
62.	$CH_3CHO + NO_3 \rightarrow HNO_3 + CH_3CO (\rightarrow CH_3C(O)O_2)$	$1.4 \times 10^{-12} e^{(-1900 / T)}$	5
63.	$CH_3CHO + O(^3P) \rightarrow OH + CH_3CO (\rightarrow CH_3C(O)O_2)$	$1.8 \times 10^{-11} e^{(-1100 / T)}$	5
64.	$CH_3CHO + OH \rightarrow H_2O + CH_3CO (\rightarrow CH_3C(O)O_2)$	$5.6 \times 10^{-12} e^{(270 / T)}$	5
65.	$O(^3P) + H_2 \rightarrow OH + H$	4.11×10^{-18}	4
66.	$NO + CH_3C(O)O_2 \rightarrow NO_2 + CH_3 + CO_2$	$5.3 \times 10^{-12} e^{(360 / T)}$	5
67.	$OH + C_2H_5OOH \rightarrow C_2H_4OOH + H_2O$	3.64×10^{-12}	4
68.	$OH + C_2H_5OOH \rightarrow C_2H_5O_2 + H_2O$	5.95×10^{-12}	4
69.	$NO_2 + O(^3P) \rightarrow NO + O_2$	$6.5 \times 10^{-12} e^{(120 / T)}$	5
70.	$NO_3 + O(^3P) \rightarrow NO_2 + O_2$	1×10^{-11}	5
71.	$HNO_3 + O(^3P) \rightarrow NO_3 + OH$	3×10^{-17}	5,b
71.	$C_2H_5O + O_2 \rightarrow CH_3CHO + HO_2$	$6.3 \times 10^{-14} e^{(-550 / T)}$	5
73.	$HO_2CH_2O \rightarrow HO_2 + CH_2O$	$2.4 \times 10^{12} e^{(-7000 / T)}$	4
74.	$HO_2CH_2O + HO_2 \rightarrow HCOOH + O_2 + H_2O$	$5.6 \times 10^{-15} e^{(2300 / T)}$	4
	Halogen chemistry		
75.	$I + O_3 \rightarrow IO + O_2$	$2 \times 10^{-11} e^{(-890 / T)}$	5
76.	$I + HO_2 \rightarrow HI + O_2$	$1.5 \times 10^{-11} e^{(-1190 / T)}$	5
77.	$IO + NO \rightarrow I + NO_2$	$7.3 \times 10^{-12} e^{(330 / T)}$	5
78.	$IO + HO_2 \rightarrow HOI + O_2$	5.8×10^{-11}	5
79.	$IO + IO \rightarrow OIO + I / I_2O_2$	8.6×10^{-11}	5
80.	$IO + OIO (+M) \rightarrow I_2O_3$	1.5×10^{-11}	5
81.	$IONO_2 \rightarrow IO + NO_2$	$2.07 \times 10^{15} e^{(-11859 / T)}$	5

82.	$OH + HI \rightarrow I + H_2O$	3×10^{-11}	5
83.	$HOI + OH \rightarrow IO + H_2O$	2×10^{-13}	5
84.	$IO + DMS \rightarrow$ Products	1.2×10^{-14}	5
85.	$INO_2 \rightarrow I + NO_2$	$(2.4 / 0.005) \times 2.07 \times 10^{15}\ e^{(-11859 / T)}$	5
86.	$Br + O_3 \rightarrow BrO + O_2$	$1.7 \times 10^{-11} e^{(-800/T)}$	5
87.	$HBr + OH \rightarrow Br + H_2O$	1.1×10^{-11}	5
88.	$Br + HO_2 \rightarrow HBr + O_2$	$1.5 \times 10^{-11} e^{(-600/T)}$	5
89.	$Br + HCHO \rightarrow HBr + HCO$	$7.7 \times 10^{-13}\ e^{(-580/T)}$	5
90.	$Br + CH_3CHO \rightarrow HBr\ CH_3CO$	$1.8 \times 10^{-12}\ e^{(-460/T)}$	5
91.	$BrO + HO_2 \rightarrow HOBr + O_2$	$3.4 \times 10^{-12} e^{(540/T)}$	5
92.	$BrO + NO \rightarrow Br + NO_2$	$8.8 \times 10^{-12} e^{(260/T)}$	5
93.	$BrO + CH_3SCH_3 \rightarrow CH_3SOCH_3 + Br$	$1.5 \times 10^{-14} e^{(850/T)}$	5
94.	$BrO + BrO \rightarrow 2Br + O_2$	$2.4 \times 10^{-12} e^{(40/T)}$	5
95.	$BrO + BrO \rightarrow Br_2 + O_2$	$2.8 \times 10^{-14} e^{(860/T)}$	5
96.	$BrONO_2 \rightarrow BrO + NO_2$	$2.8 \times 10^{13}\ e^{-(12360/T)}$	7
97.	$BrO + IO \rightarrow Br + I + O_2$ / $Br + OIO$	$1.5 \times 10^{-12} e^{(510/T)}$	5
98.	$Cl + CH_4 \rightarrow HCl + CH_3$	$1.1 \times 10^{-11} e^{(-1400/T)}$	5
99.	$HCl + OH \rightarrow H_2O + Cl$	$2.6 \times 10^{-12} e^{(-350/T)}$	5
100.	$Cl + O_3 \rightarrow ClO + O_2$	$2.9 \times 10^{-11} e^{(-260/T)}$	5
101.	$ClO + HO_2 \rightarrow HOCl + O_2$	$5.0 \times 10^{-12} e^{(700/T)}$	5
102.	$ClO + NO \rightarrow Cl + NO_2$	$6.4 \times 10^{-12} e^{(290/T)}$	5
103.	$ClO + IO \rightarrow 0.2\ (I + Cl + O_2)$	$1.3 \times 10^{-12} e^{(280/T)}$	5
104.	$Cl + Alkanes \rightarrow HCl + CH_3OO$	$5.7 \times 10^{-11} e^{(-90/T)}$	5,4
105.	$Cl + Alkenes \rightarrow HCl + CH_3OO$	1.0×10^{-10}	5.4
106.	$Cl + HCHO \rightarrow HCl + HO_2 + CO$	$7.3 \times 10^{-11}\ e^{(-30/T)}$	5
107.	$ClO + CH_3OO \rightarrow Cl + HCHO + HO_2$	$2.2 \times 10^{-12}\ e^{(-115/T)}$	5
108.	$ClO + ClO \rightarrow Cl_2O_2$	3.5×10^{-13}	5
109.	$Cl_2O_2 \rightarrow ClO + ClO$	50	5
110.	$ClONO_2 \rightarrow ClO + NO_2$	0.0022	5
111.	$Cl + ClONO_2 \rightarrow Cl_2 + NO_3$	$9.6 \times 10^{-12}\ e^{(140/T)}$	5
112.	$Cl + H_2O_2 \rightarrow HCl + HO_2$	$4.1 \times 10^{-13} e^{(-980/T)}$	5
113.	$Br_2 + Cl \rightarrow BrCl + Br$	$1.2 \times 10^{-10} e^{(-260/T)}$	5,4
114.	$BrCl + Br \rightarrow Br_2 + Cl$	3.3×10^{-15}	5.4
115.	$Cl_2 + Br \rightarrow BrCl + Cl$	1.1×10^{-15}	5,4
116.	$BrCl + Cl \rightarrow Cl_2 + Br$	1.5×10^{-11}	5.4
117.	$ClO + BrO \rightarrow Br + OClO$	$6.0 \times 10^{-12} e^{(550/T)}$	5,4
118.	$ClO + BrO \rightarrow Br + Cl + O_2$	$5.6 \times 10^{-12} e^{(260/T)}$	5.4
119.	$ClO + BrO \rightarrow BrCl + O_2$	$1.1 \times 10^{-12} e^{(290/T)}$	5,4
	Recombination Reactions		
1.	$O(^1D) + N_2\ (+M) \rightarrow N_2O\ (+M)$	$[M] \times 3.5 \times 10^{-37} \times (T / 300)^{-0.6}$	5
2.	$HO_2 + HO_2\ (+M) \rightarrow H_2O_2\ (+M)$	$[M] \times 1.7 \times 10^{-33}\ e^{(1000 / T)}$	5
3.	$H + O_2\ (+ M) \rightarrow HO_2\ (+ M)$	$k_0 = 5.7 \times 10^{-32} \times (T / 300)^{-1.6}$ $k_\infty = 7.5 \times 10^{-11}$	5
4.	$O_2 + O(^3P) \rightarrow O_3$	$[M] \times 6 \times 10^{-34} \times (T / 300)^{-2.3}$	5
5.	$NO_2 + OH \rightarrow HNO_3$	$k_0 = 2.5 \times 10^{-30} \times (T / 300)^{-4.4}$	5

		$k_\infty = 1.6 \times 10^{-11} \times (T / 300)^{-1.7}$	
6.	$NO + OH (+ M) \rightarrow HONO (+ M)$	$k_0 = 7 \times 10^{-31} \times (T / 300)^{-2.6}$	5
		$k_\infty = 1.5 \times 10^{-11} \times (T / 300)^{-0.5}$	
7.	$HO_2 + NO_2 (+ M) \rightarrow HO_2NO_2 (+ M)$	$k_0 = 1.8 \times 10^{-31} \times (T / 300)^{-3.2}$	5
		$k_\infty = 4.7 \times 10^{-12} \times (T / 300)^{-1.4}$	
8.	$HO_2NO_2 \rightarrow HO_2 + NO_2$	$k_R = k_F / k_{EQ}$	5
		$k_R = k_F / (2.1 \times 10^{-27} e^{(10900 / T)})$	
9.	$O_2 + CH_3 (+ M) \rightarrow CH_3O_2 (+ M)$	$k_0 = 4.5 \times 10^{-31} \times (T / 300)^{-3}$	5
		$k_\infty = 1.8 \times 10^{-12} \times (T / 300)^{-1.7}$	
10.	$NO_2 + NO_3 (+ M) \rightarrow N_2O_5 (+ M)$	$k_0 = 2.2 \times 10^{-30} \times (T / 300)^{-3.9}$	5
		$k_\infty = 1.5 \times 10^{-12} \times (T / 300)^{-0.7}$	
11.	$N_2O_5 (+ N_2) \rightarrow NO_2 + NO_3 (+ N_2)$	$k_R = k_F / k_{EQ}$	5
		$k_R = k_F / (2.7 \times 10^{-27} e^{(11000 / T)})$	
12.	$OH + OH (+ M) \rightarrow H_2O_2 (+ M)$	$k_0 = 6.2 \times 10^{-31} \times (T / 300)^{-1}$	5
		$k_\infty = 2.6 \times 10^{-11}$	
13.	$NO + O(^3P) (+ M) \rightarrow NO_2 (+ M)$	$k_0 = 9 \times 10^{-32} \times (T / 300)^{-1.5}$	5
		$k_\infty = 3 \times 10^{-11}$	
14.	$NO_2 + O(^3P) (+ M) \rightarrow NO_3 (+ M)$	$k_0 = 9 \times 10^{-32} \times (T / 300)^{-2}$	5
		$k_\infty = 2.2 \times 10^{-11}$	
15.	$SO_2 + OH (+ M) \rightarrow HOSO_2 (+ M)$	$k_0 = 3 \times 10^{-31} \times (T / 300)^{-3.3}$	5
		$k_\infty = 1.5 \times 10^{-12}$	
16.	$CH_3C(O)O_2 + NO_2 (+ M) \rightarrow PAN (+ M)$	$k_0 = 9.7 \times 10^{-29} \times (T / 300)^{-5.6}$	5
		$k_\infty = 9.3 \times 10^{-12} \times (T / 300)^{-1.5}$	
17.	$PAN (+ M) \rightarrow CH_3C(O)O_2 + NO_2 (+ M)$	$k_R = k_F / k_{EQ}$	5
		$k_R = k_F / (9 \times 10^{-29} e^{(14000 / T)})$	
18.	$OH + Alkenes (+ M) \rightarrow HOCH_2CH_2 (+ M)$	$k_0 = 1.5 \times 10^{-28} \times (T / 300)^{-0.8}$	5,4
		$k_\infty = 8.8 \times 10^{-12}$	
19.	$C_2H_5 + O_2 (+ M) \rightarrow C_2H_5O_2 (+ M)$	$k_0 = 1.5 \times 10^{-28} \times (T / 300)^{-3.8}$	5
		$k_\infty = 8 \times 10^{-12}$	
20.	$NO_2 + CH_3O_2 (+ M) \rightarrow CH_3O_2NO_2 (+ M)$	$k_0 = 1.5 \times 10^{-30} \times (T / 300)^{-4}$	5
		$k_\infty = 6.5 \times 10^{-12} \times (T / 300)^{-2}$	
21.	$CH_3O_2NO_2 \rightarrow CH_3O_2 + NO_2$	$k_R = k_F / k_{EQ}$	5
		$k_R = k_F / (1.3 \times 10^{-28} e^{(11200 / T)})$	
22.	$I + NO_2 (+ M) \rightarrow INO_2 (+ M)$	$k_0 = 3 \times 10^{-31} \times (T / 300)^{-1}$	5
		$k_\infty = 6.6 \times 10^{-11}$	
		$F_c = e^{(-T / 650)} + e^{(-2600 / T)}$	
23.	$IO + NO_2 (+ M) \rightarrow IONO_2 (+ M)$	$k_0 = 7.7 \times 10^{-31} \times (T / 300)^{-5}$	5
		$k_\infty = 1.6 \times 10^{-11}$	
		$F_c = 0.4$	
24.	$Br + NO_2 + M \rightarrow BrNO_2$	$k_0 = 4.2 \times 10^{-31} \times (T / 300)^{-2.4}$	5
		$k_\infty = 2.7 \times 10^{-11} \times (T / 300)^{-0}$	
25.	$BrO + NO_2 + M \rightarrow BrONO_2$	$k_0 = 5.2 \times 10^{-31} \times (T / 300)^{-3.2}$	5
		$k_\infty = 6.9 \times 10^{-12} \times (T / 300)^{-2.9}$	
25.	$ClO + NO_2 + M \rightarrow ClONO_2$	$k_0 = 1.6.2 \times 10^{-31} \times (T / 300)^{-3.4}$	5
		$k_\infty = 1.5 \times 10^{-11}$	

	Photochemical Reactions	References
J1.	$O_3 + h\nu \rightarrow O_2 + O(^1D)$	5,4,c
J2.	$H_2O_2 + h\nu \rightarrow 2OH$	5,4,c
J3.	$HNO_3 + h\nu \rightarrow OH + NO_2$	5,4,c
J4.	$HO_2NO_2 + h\nu \rightarrow OH + NO_3$	5,4,c
J5.	$HONO + h\nu \rightarrow OH + NO$	5,4,c
J6.	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	5,4,c
J7.	$CH_2O + h\nu \rightarrow HCO + H$	5,4,c
J8.	$CH_2O + h\nu \rightarrow CO + H_2$	5,4,c
J9.	$NO_2 + h\nu \rightarrow NO + O$	5,4,c
J10.	$NO_3 + h\nu \rightarrow NO_2 + O$	5,4,c
J11.	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	5,4,c
J12.	$C_2H_5O_2H + h\nu \rightarrow OH + C_2H_5O$	5,4,c
J13.	$CH_3CHO + h\nu \rightarrow CH_3 + HCO$	5,4,c
J15.	PAN ($CH3C(O)O_2NO_2$) + $h\nu \rightarrow CH_3C(O)O_2 + NO_2$	5,4,c
J16.	$NO_3 + h\nu \rightarrow NO + O_2$	5,4,c
J17.	$CH_3I + h\nu \rightarrow CH_3 + I$	5,4,c
J18.	$CH_2I_2 + h\nu \rightarrow CH_2I + I \rightarrow CH_2 + 2I$	5,4,c
J19.	$CH_2IBr + h\nu \rightarrow CH_2Br + I$	5,4,c
J20.	$I_2 + h\nu \rightarrow 2I$	5,4,c
J21.	$INO_2 + h\nu \rightarrow I + NO_2$ / IO + NO	5,4,c
J22.	$IO + h\nu \rightarrow I + O$	5,4,c
J23.	$OIO + h\nu \rightarrow I + O_2$	5,4,c
J24.	$IONO_2 + h\nu \rightarrow I + NO_3$	5,4,c
J25.	$HOI + h\nu \rightarrow I + OH$	5,4,c
J26.	$BrO + h\nu \rightarrow Br + O$	5,4,c
J27.	$Br_2 + h\nu \rightarrow 2Br$	5,4,c
J28.	$IBr + h\nu \rightarrow Br + I$	5,4,c
J29.	$BrCl + h\nu \rightarrow Br + Cl$	5,4,c
J30.	$BrNO_2 + h\nu \rightarrow Br + NO_2$	5,4,c
J31.	$BrONO_2 + h\nu \rightarrow 0.7\ (BrO + NO_2) / 0.3\ (Br + NO_3)$	5,4,c
J32.	$HOBr + h\nu \rightarrow Br + OH$	5,4,c
J33.	$Cl_2 + h\nu \rightarrow 2Cl$	5,4,c
J34.	$ICl + h\nu \rightarrow I + Cl$	5,4,c
J35.	$ClO + h\nu \rightarrow Cl + O$	5,4,c
J36.	$HOCl + h\nu \rightarrow Cl + OH$	5,4,c
J37.	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	5,4,c
J38.	$ClONO_2 + h\nu \rightarrow 0.9\ (Cl + NO_3) / 0.1\ (ClO + NO_2)$	5,4,c

Species	Deposition velocities, cm s^{-1}	References
HOI	1.0	8
HOBr	1.0	d
HOCl	1.0	d
HBr	2.0	d
HCl	2.0	d
HI	1.0	8
$BrONO_2$	1.0	d
$IONO_2$	1.0	8
$ClONO_2$	1.0	d
INO_2	1.0	d

[a]Units: unimolecular reactions, s^{-1}; photolysis rate constants, s^{-1}; bimolecular reactions, cm^3 $molecule^{-1}$ s^{-1}; termolecular reactions, cm^6 $molecule^{-2}$ s^{-1}, calculated using the formalism of *Sander et al.* (2006), where $k = ((k_o\,[M]/(1 + k_o[M]/k_\infty)) \times F_c^n)$, $F_c = 0.6$ (unless otherwise noted) and $n = (1 + (\log_{10}(k_o[M]/k_\infty))^2)^{-1}$.

[b]set as upper limit.

[c]absorption cross-sections taken from *Atkinson et al*., 2000.

[d]deposition velocities estimated.

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