Kinetic data for MISTRA

supplemental material to:

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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 7).

Table 1: Species

Gas phase
O^1D, O_2, O_3, OH, HO_2, H_2O_2, H_2O
NO, NO_2, NO_3, N_2O_5, HONO, HNO_3, HNO_4, PAN, NH_3
CO, CO_2, CH_4, C_2H_6, C_2H_4, HCHO, HCOOH, ALD, CH_2O_2, $HOCH_2O_2$, CH_3CO_3, CH_3O_2, $C_2H_5O_2$, EO_2, CH_2O_2, ROOH
SO_2, SO_3, $HOSO_2$, H_2SO_4, DMS, CH_3SCH_2OO, DMSO, $DMSO_2$, CH_3S, CH_3SO, CH_3SO_2, CH_3SO_3, CH_3SO_2H, CH_3SO_3H
Cl, ClO, OClO, HCl, HOCl, Cl_2, Cl_2O_2 $ClNO_2$, $ClNO_3$
Br, BrO, HBr, HOBr, Br_2, $BrNO_2$, $BrNO_3$, BrCl
I, IO, OIO, HI, HOI, INO_2, INO_3, I_2, ICl, IBr, HIO_3, CH_3I, C_2H_5I, C_3H_7I, CH_2ClI, CH_2BrI, CH_2I_2
Liquid phase (neutral)
O_2, O_3, OH, HO_2, H_2O_2, H_2O
NO, NO_2, NO_3, HONO, HNO_3, HNO_4, NH_3
CO_2, HCHO, HCOOH, CH_3OH, CH_3OO, CH_3OOH
SO_2, H_2SO_4, DMSO, $DMSO_2$, CH_3SO_2H, CH_3SO_3H
Cl, HCl, HOCl, Cl_2
Br, HBr, HOBr, Br_2, BrCl
IO, HI, HOI, I_2, ICl, IBr
Liquid phase (ions)
H^+, OH^-, O_2^-
NO_2^-, NO_3^-, NO_4^-, NH_4^+
HCO_3^-, CO_3^-, $HCOO^-$
HSO_3^-, $SO_3{}^2-$, HSO_4^-, SO_4^{2-}, HSO_5^-, SO_3^-, SO_4^-, SO_5^-, $CH_3SO_3^-$, $CH_2OHSO_2^-$, $CH_2OHSO_3^-$
Cl^-, Cl_2^-, ClO^-, $ClOH^-$
Br^-, Br_2^-, BrO^-, $BrCl_2^-$, Br_2Cl^-, $BrOH^-$
I^-, IO_2^-, IO_3^-, ICl_2^-, IBr_2^-, $IClBr^-$

Table 2: Gas phase reactions.

no	reaction	n	A [$(cm^{-3})^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
O 1	$O^1D + O_2 \longrightarrow O_3$	2	3.2×10^{-11}	70	Atkinson et al. (2004)
O 2	$O^1D + N_2 \longrightarrow O_3$	2	1.8×10^{-11}	110	Atkinson et al. (2004)
O 3	$O^1D + H_2O \longrightarrow 2\ OH$	2	2.2×10^{-10}		Atkinson et al. (2004)
O 4	$OH + O_3 \longrightarrow HO_2 + O_2$	2	1.7×10^{-12}	-940	Atkinson et al. (2004)
O 5	$OH + HO_2 \longrightarrow H_2O + O_2$	2	4.8×10^{-11}	250	Atkinson et al. (2004)
O 6	$OH + H_2O_2 \longrightarrow HO_2 + H_2O$	2	2.9×10^{-12}	-160	Atkinson et al. (2004)
O 7	$HO_2 + O_3 \longrightarrow OH + 2O_2$	2	1.0×10^{-14}	-490	Atkinson et al. (2004)
O 8	$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$	2	2.3×10^{-13}	600	Atkinson et al. (2004)
O 9	$O_3 + h\nu \longrightarrow O_2 + O^1D$	1	[1]		DeMore et al. (1997)
O 10	$H_2O_2 + h\nu \longrightarrow 2OH$	1	[1]		DeMore et al. (1997)
N 1	$NO + OH \xrightarrow{M} HONO$	3	[2]		Sander et al. (2003)
N 2	$NO + HO_2 \longrightarrow NO_2 + OH$	2	3.5×10^{-12}	250	Atkinson et al. (2004)
N 3	$NO + O_3 \longrightarrow NO_2 + O_2$	2	3.0×10^{-12}	-1500	Sander et al. (2003)
N 4	$NO + NO_3 \longrightarrow 2NO_2$	2	1.5×10^{-11}	170	Sander et al. (2003)
N 5	$NO_2 + OH \xrightarrow{M} HNO_3$	3	[2]		Sander et al. (2003)
N 6	$NO_2 + HO_2 \xrightarrow{M} HNO_4$	3	[2]		Atkinson et al. (2004)
N 7	$NO_2 + O_3 \longrightarrow NO_3 + O_2$	2	1.2×10^{-13}	-2450	Sander et al. (2003)
N 8	$NO_2 + h\nu \longrightarrow NO + O_3$	1	[1]		DeMore et al. (1997)
N 9	$NO_2 + NO_3 \xrightarrow{M} N_2O_5$	3	[2]		Sander et al. (2003)
N 10	$NO_3 + h\nu \longrightarrow NO + O_2$	1	[1]		Wayne et al. (1991)
N 11	$NO_3 + HO_2 \longrightarrow 0.3\ HNO_3 + 0.7\ OH + 0.7\ NO_2 + O_2$	2	4.0×10^{-12}		Atkinson et al. (2004)
N 12	$NO_3 + NO_3 \longrightarrow NO_2 + NO_2 + O_2$	2	8.5×10^{-13}	-2450	Sander et al. (2003)
N 13	$NO_3 + h\nu \longrightarrow NO_2 + O_3$	1	[1]		Wayne et al. (1991)
N 14	$N_2O_5 \xrightarrow{M} NO_2 + NO_3$	2	[2]		Sander et al. (2003)
N 15	$N_2O_5 + H_2O \longrightarrow 2HNO_3$	2	2.6×10^{-22}		Atkinson et al. (2004)
N 16	$N_2O_5 + h\nu \longrightarrow NO_2 + NO_3$	1	[1]		DeMore et al. (1997)
N 17	$HONO + OH \longrightarrow NO_2$	2	1.8×10^{-11}	-390	Sander et al. (2003)
N 18	$HONO + h\nu \longrightarrow NO + OH$	1	[1]		DeMore et al. (1997)
N 19	$HNO_3 + h\nu \longrightarrow NO_2 + OH$	1	[1]		DeMore et al. (1997)
N 20	$HNO_3 + OH \longrightarrow NO_3 + H_2O$	2	[2]		Atkinson et al. (2004)
N 21	$HNO_4 \xrightarrow{M} NO_2 + HO_2$	2	[2]		Sander et al. (2003)
N 22	$HNO_4 + OH \longrightarrow NO_2 + H_2O + O_2$	2	1.3×10^{-12}	380	Haggerstone et al. (2005)
N 23	$HNO_4 + h\nu \longrightarrow NO_2 + HO_2$	1	[1]		DeMore et al. (1997)
N 24	$HNO_4 + h\nu \longrightarrow OH + NO_3$	1	[1]		DeMore et al. (1997)

Table 2: Continued.

no	reaction	n	A [$(\mathrm{cm}^{-3})^{1-n}\mathrm{s}^{-1}$]	$-E_a$ / R [K]	reference
C 1	$CO + OH \xrightarrow{O_2} HO_2 + CO_2$	2	[2]		Sander et al. (2003)
C 2	$CH_4 + OH \xrightarrow{O_2} CH_3OO + H_2O$	2	2.4×10^{-12}	-1775	Sander et al. (2003)
C 3	$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	2	1.7×10^{-11}	-1232	Lurmann et al. (1986)
C 4	$C_2H_4 + OH \longrightarrow EO_2$	2	1.66×10^{-12}	474	Lurmann et al. (1986), see note
C 5	$C_2H_4 + O_3 \longrightarrow HCHO + 0.4CH_2O_2 + 0.12HO_2 + 0.42CO + 0.06CH_4$	2	1.2×10^{-14}	-2633	Lurmann et al. (1986), see note
C 6	$HO_2 + CH_3OO \longrightarrow ROOH + O_2$	2	4.1×10^{-13}	750	Sander et al. (2003)
C 7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	7.5×10^{-13}	700	Sander et al. (2003)
C 8	$HO_2 + CH_3CO_3 \longrightarrow ROOH + O_2$	2	4.5×10^{-13}	1000	DeMore et al. (1997)
C 9	$CH_3OO + CH_3OO \longrightarrow 1.4HCHO + 0.8HO_2 + O_2$	2	1.5×10^{-13}	220	Lurmann et al. (1986)
C 10	$C_2H_5O_2 + NO \longrightarrow ALD + HO_2 + NO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 11	$2C_2H_5O_2 \longrightarrow 1.6ALD + 1.2HO_2$	2	5.00×10^{-14}		Lurmann et al. (1986)
C 12	$EO_2 + NO \longrightarrow NO_2 + 2.0HCHO + HO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 13	$EO_2 + EO_2 \longrightarrow 2.4HCHO + 1.2HO_2 + 0.4ALD$	2	5.00×10^{-14}		Lurmann et al. (1986)
C 14	$HO_2 + EO_2 \longrightarrow ROOH + O_2$	2	3.00×10^{-12}		Lurmann et al. (1986)
C 15	$HCHO + h\nu \longrightarrow 2HO_2 + CO$	1	[1]		DeMore et al. (1997)
C 16	$HCHO + h\nu \longrightarrow CO + H_2$	1	[1]		DeMore et al. (1997)
C 17	$HCHO + OH \xrightarrow{O_2} HO_2 + CO + H_2O$	2	1.00×10^{-11}		DeMore et al. (1997)
C 18	$HCHO + HO_2 \longrightarrow HOCH_2O_2$	2	6.7×10^{-15}	600	Sander et al. (2003)
C 19	$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	2	5.8×10^{-16}		DeMore et al. (1997)
C 20	$ALD + OH \longrightarrow CH_3CO_3 + H_2O$	2	6.9×10^{-12}	250	Lurmann et al. (1986)
C 21	$ALD + NO_3 \longrightarrow HNO_3 + CH_3CO_3$	2	1.40×10^{-15}		DeMore et al. (1997)
C 22	$ALD + h\nu \longrightarrow CH_3OO + HO_2 + CO$	1	[1]		Lurmann et al. (1986)
C 23	$ALD + h\nu \longrightarrow CH_4 + CO$	1	[1]		Lurmann et al. (1986)
C 24	$HOCH_2O_2 + NO \longrightarrow HCOOH + HO_2 + NO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 25	$HOCH_2O_2 + HO_2 \longrightarrow HCOOH + H_2O + O_2$	2	2.00×10^{-12}		Lurmann et al. (1986)
C 26	$2\ HOCH_2O_2 \longrightarrow 2HCOOH + 2HO_2 + 2O_2$	2	1.00×10^{-13}		Lurmann et al. (1986)
C 27	$HCOOH + OH \xrightarrow{O_2} HO_2 + H_2O + CO_2$	2	4.0×10^{-13}		DeMore et al. (1997)
C 28	$CH_3CO_3 + NO_2 \longrightarrow PAN$	2	4.70×10^{-12}		Lurmann et al. (1986)
C 29	$PAN \longrightarrow CH_3CO_3 + NO_2$	1	1.9×10^{16}	-13543	DeMore et al. (1997)
C 30	$CH_3CO_3 + NO \longrightarrow CH_3OO + NO_2 + CO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 31	$CH_3OO + NO \xrightarrow{O_2} HCHO + NO_2 + HO_2$	2	3.0×10^{-12}	280	DeMore et al. (1997)
C 32	$ROOH + OH \longrightarrow 0.7\ CH_3OO + 0.3\ HCHO + 0.3\ OH$	2	3.8×10^{-12}	200	DeMore et al. (1997), see note
C 33	$ROOH + h\nu \longrightarrow HCHO + OH + HO_2$	1	[1]		DeMore et al. (1997), see note

Table 2: Continued.

no	reaction	n	A [(cm^{-3})$^{1-n}$s^{-1}]	$-E_a$ / R [K]	reference
S 1	$SO_2 + OH \xrightarrow{M} HOSO_2$	3	^{2}		Atkinson et al. (2004)
S 2	$HOSO_2 + O_2 \longrightarrow HO_2 + SO_3$	2	1.3×10^{-12}	330	Atkinson et al. (2004)
S 3	$SO_3 \xrightarrow{H_2O} H_2SO_4$	1	^{2}		Jayne et al. (1997)
S 4	$CH_3SCH_3 + OH \longrightarrow CH_3SCH_2OO + H_2O$	2	^{2}		Atkinson et al. (1997)
S 5	$CH_3SCH_3 + OH \xrightarrow{O_2} CH_3SOCH_3 + HO_2$	2	^{2}		Atkinson et al. (1997)
S 6	$CH_3SCH_3 + NO_3 \xrightarrow{O_2} CH_3SCH_2OO + HNO_3$	2	1.9×10^{-13}	520	Atkinson et al. (1999)
S 7	$CH_3SCH_3 + Cl \xrightarrow{O_2} CH_3SCH_2OO + HCl$	2	3.3×10^{-10}		Atkinson et al. (1999)
S 8	$CH_3SCH_3 + Br \xrightarrow{O_2} CH_3SCH_2OO + HBr$	2	9.0×10^{-11}	-2386	Jefferson et al. (1994)
S 9	$CH_3SCH_3 + BrO \longrightarrow CH_3SOCH_3 + Br$	2	2.54×10^{-14}	850	Ingham et al. (1999)
S 10	$CH_3SCH_3 + ClO \longrightarrow CH_3SOCH_3 + Cl$	2	9.5×10^{-15}		Barnes et al. (1991)
S 11	$CH_3SCH_3 + IO \longrightarrow CH_3SOCH_3 + I$	2	1.4×10^{-14}		THALOZ (2005)
S 12	$CH_3SCH_2OO + NO \longrightarrow HCHO + CH_3S + NO_2$	2	4.9×10^{-12}	263	Urbanski et al. (1997)
S 13	$CH_3SCH_2OO + CH_3SCH_2OO \xrightarrow{O_2} 2\ HCHO + 2\ CH_3S$	2	1.0×10^{-11}		Urbanski et al. (1997); Atkinson et al. (2004)
S 14	$CH_3S + O_3 \longrightarrow CH_3SO + O_2$	2	1.15×10^{-12}	432	Atkinson et al. (2004)
S 15	$CH_3S + NO_2 \longrightarrow CH_3SO + NO$	2	3.0×10^{-11}	210	Atkinson et al. (2004)
S 16	$CH_3SO + NO_2 \xrightarrow{O_2} 0.82\ CH_3SO_2 + 0.18\ SO_2 + 0.18\ MO_2 + NO$	2	1.2×10^{-11}		Atkinson et al. (2004); Kukui et al. (2000), product ratios from van Dingenen et al. (1994)
S 17	$CH_3SO + O_3 \xrightarrow{O_2} CH_3SO_2$	2	6.0×10^{-13}		Atkinson et al. (2004)
S 18	$CH_3SO_2 \longrightarrow SO_2 + CH_3OO$	1	1.9×10^{13}	-8661	Barone et al. (1995)
S 19	$CH_3SO_2 + NO_2 \longrightarrow CH_3SO_3 + NO$	2	2.2×10^{-12}		Ray et al. (1996)
S 20	$CH_3SO_2 + O_3 \longrightarrow CH_3SO_3$	2	$3.\ \times10^{-13}$		Barone et al. (1995)
S 21	$CH_3SO_3 + HO_2 \longrightarrow CH_3SO_3H$	2	$5.\ \times10^{-11}$		Barone et al. (1995)
S 22	$CH_3SO_3 \xrightarrow{H_2O,O_2} CH_3OO + H_2SO_4$	1	1.36×10^{14}	-11071	Barone et al. (1995)
S 23	$CH_3SOCH_3 + OH \longrightarrow 0.95\ CH_3SO_2H + 0.95\ CH_3OO + 0.05\ DMSO_2$	2	8.7×10^{-11}		Urbanski et al. (1998)
S 24	$CH_3SO_2H + OH \longrightarrow 0.95\ CH_3SO_2 + 0.05\ CH_3SO_3H + 0.05\ HO_2 + H_2O$	2	$9.\times10^{-11}$		Kukui et al. (2003)
S 25	$CH_3SO_2H + NO_3 \longrightarrow CH_3SO_2 + HNO_3$	2	1.0×10^{-13}		Yin et al. (1990)

Table 2: Continued.

no	reaction	n	A [(cm^{-3})$^{1-n}$s^{-1}]	$-E_a$ / R [K]	reference
Cl 1	$Cl + O_3 \longrightarrow ClO + O_2$	2	2.8×10^{-11}	-250	Atkinson et al. (2004)
Cl 2	$Cl + HO_2 \longrightarrow HCl + O_2$	2	1.8×10^{-11}	170	Sander et al. (2003)
Cl 3	$Cl + HO_2 \longrightarrow ClO + OH$	2	$.1 \times 10^{-11}$	-450	Sander et al. (2003)
Cl 4	$Cl + H_2O_2 \longrightarrow HCl + HO_2$	2	1.1×10^{-11}	-980	Atkinson et al. (2004)
Cl 5	$Cl + CH_3OO \longrightarrow 0.5\ ClO + 0.5\ HCHO + 0.5\ HO_2 + 0.5\ HCl + 0.5\ CO + 0.5\ H_2O$	2	1.6×10^{-10}		Sander et al. (2003)
Cl 6	$Cl + CH_4 \xrightarrow{O_2} HCl + CH_3OO$	2	9.6×10^{-12}	-1360	Sander et al. (2003)
Cl 7	$Cl + C_2H_6 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	7.7×10^{-11}	-90	Sander et al. (2003)
Cl 8	$Cl + C_2H_4 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	$1. \times 10^{-10}$		see note
Cl 9	$Cl + HCHO \xrightarrow{O_2} HCl + HO_2 + CO$	2	8.1×10^{-11}	-30	Sander et al. (2003)
Cl 10	$Cl + ROOH \longrightarrow CH_3OO + HCl$	2	5.7×10^{-11}		Wallington et al. (1990), see note
Cl 11	$Cl + OClO \longrightarrow ClO + ClO$	2	3.2×10^{-11}	170	Atkinson et al. (2004)
Cl 12	$Cl + ClNO_3 \longrightarrow Cl_2 + NO_3$	2	6.5×10^{-12}	135	Sander et al. (2003)
Cl 13	$ClO + OH \longrightarrow Cl + HO_2$	2	7.4×10^{-12}	-270	Sander et al. (2003)
Cl 14	$ClO + OH \longrightarrow HCl + O_2$	2	6.0×10^{-13}	-230	Sander et al. (2003)
Cl 15	$ClO + HO_2 \longrightarrow HOCl + O_2$	2	2.2×10^{-12}	340	Atkinson et al. (2004)
Cl 16	$ClO + CH_3OO \longrightarrow Cl + HCHO + HO_2$	2	3.3×10^{-12}	-115	Sander et al. (2003)
Cl 17	$ClO + NO \longrightarrow Cl + NO_2$	2	6.2×10^{-12}	295	Atkinson et al. (2004)
Cl 18	$ClO + NO_2 \xrightarrow{M} ClNO_3$	3	[2]		Atkinson et al. (2004)
Cl 19	$ClO + ClO \longrightarrow Cl_2O_2$	2	[2]		Atkinson et al. (2004)
Cl 20	$ClO + ClO \longrightarrow Cl_2 + O_2$	2	1.0×10^{-12}	-1590	Atkinson et al. (2004)
Cl 21	$ClO + ClO \longrightarrow Cl_2O_2$	2	3.0×10^{-11}	-2450	Atkinson et al. (2004)
Cl 22	$ClO + ClO \longrightarrow Cl + OClO$	2	3.5×10^{-13}	-1370	Atkinson et al. (2004)
Cl 23	$OClO + OH \longrightarrow HOCl + O_2$	2	4.5×10^{-13}	800	Atkinson et al. (2004)
Cl 24	$OClO + NO \longrightarrow ClO + NO_2$	2	1.1×10^{-13}	350	Atkinson et al. (2004)
Cl 25	$Cl_2O_2 \longrightarrow ClO + ClO$	1	[2]		Atkinson et al. (2004)
Cl 26	$HOCL + OH \longrightarrow ClO + H_2O$	2	3.0×10^{-12}	-500	Sander et al. (2003)
Cl 27	$HCl + OH \longrightarrow H_2O + Cl$	2	1.8×10^{-12}	-240	Atkinson et al. (2004)
Cl 28	$ClNO_2 + OH \longrightarrow HOCl + NO_2$	2	2.4×10^{-12}	-1250	Atkinson et al. (2004)
Cl 29	$ClNO_3 + OH \longrightarrow 0.5\ ClO + 0.5\ HNO_3 + 0.5\ HOCl + 0.5\ NO_3$	2	1.2×10^{-12}	-330	Atkinson et al. (2004)
Cl 30	$ClNO_3 \longrightarrow ClO + NO_2$	1	[2]		Anderson and Fahey (1990)
Cl 31	$OClO + h\nu \xrightarrow{O_2,O_3} O_3 + ClO$	1	[1]		DeMore et al. (1997)
Cl 32	$Cl_2O_2 + h\nu \longrightarrow Cl + Cl + O_2$	1	[1]		DeMore et al. (1997)
Cl 33	$Cl_2 + h\nu \longrightarrow 2\ Cl$	1	[1]		DeMore et al. (1997)
Cl 34	$HOCl + h\nu \longrightarrow Cl + OH$	1	[1]		DeMore et al. (1997)
Cl 35	$ClNO_2 + h\nu \longrightarrow Cl + NO_2$	1	[1]		DeMore et al. (1997)
Cl 36	$ClNO_3 + h\nu \longrightarrow Cl + NO_3$	1	[1]		DeMore et al. (1997)

Table 2: Continued.

no	reaction	n	A [$(cm^{-3})^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
Br 1	$Br + O_3 \longrightarrow BrO + O_2$	2	1.7×10^{-11}	-800	Atkinson et al. (2004)
Br 2	$Br + HO_2 \longrightarrow HBr + O_2$	2	7.7×10^{-12}	-450	Atkinson et al. (2004)
Br 3	$Br + C_2H_4 \xrightarrow{O_2} HBr + C_2H_5O_2$	2	$5. \times 10^{-14}$		see note
Br 4	$Br + HCHO \xrightarrow{O_2} HBr + CO + HO_2$	2	1.7×10^{-11}	-800	Sander et al. (2003)
Br 5	$Br + ROOH \longrightarrow CH_3OO + HBr$	2	2.66×10^{-12}	-1610	Mallard et al. (1993), see note
Br 6	$Br + NO_2 \longrightarrow BrNO_2$	2	[2]		Sander et al. (2003)
Br 7	$Br + BrNO_3 \longrightarrow Br_2 + NO_3$	2	4.9×10^{-11}		Orlando and Tyndall (1996)
Br 8	$BrO + OH \longrightarrow Br + HO_2$	2	1.8×10^{-11}	250	Atkinson et al. (2004)
Br 9	$BrO + HO_2 \longrightarrow HOBr + O_2$	2	4.5×10^{-12}	500	Atkinson et al. (2004)
Br 10	$BrO + CH_3OO \longrightarrow HOBr + HCHO$	2	4.1×10^{-12}		Aranda et al. (1997)
Br 11	$BrO + CH_3OO \longrightarrow Br + HCHO + HO_2$	2	1.6×10^{-12}		Aranda et al. (1997)
Br 12	$BrO + HCHO \xrightarrow{O_2} HOBr + CO + HO_2$	2	1.5×10^{-14}		Hansen et al. (1999)
Br 13	$BrO + NO \longrightarrow Br + NO_2$	2	8.7×10^{-12}	260	Atkinson et al. (2004)
Br 14	$BrO + NO_2 \xrightarrow{M} BrNO_3$	3	[2]		Atkinson et al. (2004)
Br 15	$BrO + BrO \longrightarrow 2\,Br + O_2$	2	2.4×10^{-12}	40	Sander et al. (2003)
Br 16	$BrO + BrO \longrightarrow Br_2 + O_2$	2	2.9×10^{-14}	860	Sander et al. (2003)
Br 17	$HBr + OH \longrightarrow Br + H_2O$	2	5.5×10^{-12}	205	Atkinson et al. (2004)
Br 18	$BrNO_3 \longrightarrow BrO + NO_2$	1	[2]		Orlando and Tyndall (1996)
Br 19	$BrO + h\nu \xrightarrow{O_2} Br + O_3$	1	[1]		DeMore et al. (1997)
Br 20	$Br_2 + h\nu \longrightarrow 2\,Br$	1	[1]		Hubinger and Nee (1995)
Br 21	$HOBr + h\nu \longrightarrow Br + OH$	1	[1]		Ingham et al. (1999)
Br 22	$BrNO_2 + h\nu \longrightarrow Br + NO_2$	1	[1]		Scheffler et al. (1997)
Br 23	$BrNO_3 + h\nu \longrightarrow Br + NO_3$	1	[1]		DeMore et al. (1997)

Table 2: Continued.

no	reaction	n	A [$(\mathrm{cm}^{-3})^{1-n}\mathrm{s}^{-1}$]	$-E_a$ / R [K]	reference
I 1	$I + O_3 \longrightarrow IO + O_2$	2	1.9×10^{-11}	-830	Atkinson et al. (2004)
I 2	$I + HO_2 \longrightarrow HI + O_2$	2	1.5×10^{-11}	-1090	Atkinson et al. (2004)
I 3	$I + NO_2 \xrightarrow{M} INO_2$	3	[2]		Atkinson et al. (2004)
I 4	$I + NO_3 \longrightarrow IO + NO_2$	2	4.5×10^{-10}		Chambers et al. (1992)
I 5	$I + I \longrightarrow I_2$	2	2.99×10^{-11}		Hippler et al. (1973)
I 6	$IO + HO_2 \longrightarrow HOI + O_2$	2	1.4×10^{-11}	540	Atkinson et al. (2004)
I 7	$IO + NO \longrightarrow I + NO_2$	2	7.15×10^{-12}	300	Atkinson et al. (2004)
I 8	$IO + NO_2 \xrightarrow{M} INO_3$	3	[2]		Atkinson et al. (2004)
I 9	$IO + IO \longrightarrow OIO + I$	2	5.4×10^{-11}	180	Atkinson et al. (2004), for product ratios see text
I 10	$OIO + OH \longrightarrow 0.5\ HIO_3 + 0.5\ HOI$	2	2.0×10^{-10}		assumed, see von Glasow et al. (2002b)
I 11	$OIO + NO \longrightarrow NO_2 + IO$	2	5.1×10^{-13}	712	THALOZ (2005)
I 12	$HI + OH \longrightarrow I + H_2O$	2	1.6×10^{-11}	440	Atkinson et al. (2004)
I 13	$HI + NO_3 \longrightarrow I + HNO_3$	2	1.3×10^{-12}	-1830	Atkinson et al. (2004)
I 14	$INO_2 \xrightarrow{M} I + NO_2$	2	2.4		estimated from data in Jenkin et al. (1985)
I 15	$INO_3 \xrightarrow{M} IO + NO_2$	2	1.1×10^{15}	-12060	Atkinson et al. (2005)
I 16	$I_2 + OH \longrightarrow I + HOI$	2	2.1×10^{-10}		Atkinson et al. (2004)
I 17	$I_2 + NO_3 \longrightarrow I + INO_3$	2	1.5×10^{-12}		Chambers et al. (1992)
I 18	$CH_3I + OH \longrightarrow HCHO + I$	2	4.3×10^{-12}	-1120	Atkinson et al. (2004)
I 19	$C_3H_7I + OH \longrightarrow CH_3OO + I$	2	1.2×10^{-12}		J. Crowley, pers. comm.
I 20	$IO + h\nu \xrightarrow{O_2} I + O_3$	1	[1]		Laszlo et al. (1995)
I 21	$OIO + h\nu \longrightarrow I + O_2$	1	[1]		THALOZ (2005), for sensitivity studies see text
I 22	$HOI + h\nu \longrightarrow I + OH$	1	[1]		Bauer et al. (1998)
I 23	$INO_2 + h\nu \longrightarrow I + NO_2$	1	[1]		Bröske and Zabel (1998) , R. Bröske, pers. comm.
I 24	$INO_3 + h\nu \longrightarrow I + NO_3$	1	[1]		same as $BrNO_3$, but redshifted by 50 nm
I 25	$I_2 + h\nu \longrightarrow 2\ I$	1	[1]		Wesely (1989)
I 26	$CH_3I + h\nu \longrightarrow I + CH_3OO$	1	[1]		Roehl et al. (1997)
I 27	$C_2H_5I + h\nu \longrightarrow I + ROOH$	1	[1]		= CH_3I
I 28	$C_3H_7I + h\nu \longrightarrow I + ROOH$	1	[1]		Roehl et al. (1997)
I 29	$CH_2ClI + h\nu \longrightarrow I + Cl + 2\ HO_2 + CO$	1	[1]		Roehl et al. (1997)
I 30	$CH_2BrI + h\nu \longrightarrow I + Br + 2\ HO_2 + CO$	1	[1]		Mössinger et al. (1998)
I 31	$CH_2I_2 + h\nu \longrightarrow I + IO + HCHO$	1	[1]		Roehl et al. (1997)

Table 2: Continued.

no	reaction	n	A [$(cm^{-3})^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
Hx 1	$Cl + CH_3I \longrightarrow HCl + HCHO + I$	2	2.9×10^{-11}	-1000	Sander et al. (2003), products simplified
Hx 2	$Cl + BrCl \longrightarrow Br + Cl_2$	2	1.5×10^{-11}		Mallard et al. (1993)
Hx 3	$Cl + Br_2 \longrightarrow BrCl + Br$	2	1.2×10^{-10}		Mallard et al. (1993)
Hx 4	$I_2 + Cl \longrightarrow I + ICl$	2	2.09×10^{-10}		Bedjanian et al. (1996)
Hx 5	$Br + OClO \longrightarrow BrO + ClO$	2	2.6×10^{-11}	-1300	Atkinson et al. (2004)
Hx 6	$Br + Cl_2 \longrightarrow BrCl + Cl$	2	1.1×10^{-15}		Mallard et al. (1993)
Hx 7	$Br + BrCl \longrightarrow Br_2 + Cl$	2	3.3×10^{-15}		Mallard et al. (1993)
Hx 8	$I_2 + Br \longrightarrow I + IBr$	2	1.2×10^{-10}		Bedjanian et al. (1997)
Hx 9	$I + BrO \longrightarrow IO + Br$	2	1.2×10^{-11}		Sander et al. (2003)
Hx 10	$BrO + ClO \longrightarrow Br + OClO$	2	1.6×10^{-12}	430	Atkinson et al. (2004)
Hx 11	$BrO + ClO \longrightarrow Br + Cl + O_2$	2	2.9×10^{-12}	220	Atkinson et al. (2004)
Hx 12	$BrO + ClO \longrightarrow BrCl + O_2$	2	5.8×10^{-13}	170	Atkinson et al. (2004)
Hx 13	$IO + ClO \longrightarrow 0.8\ I + 0.55\ OClO + 0.45\ O_2 + 0.25\ Cl + 0.2\ ICl$	2	4.7×10^{-12}	280	Atkinson et al. (2004)
Hx 14	$IO + BrO \longrightarrow Br + 0.8\ OIO + 0.2\ I + 0.2\ O_2$	2	1.5×10^{-11}	510	Atkinson et al. (2004)
Hx 15	$BrCl + h\nu \longrightarrow Br + Cl$	1	[1]		DeMore et al. (1997)
Hx 16	$ICl + h\nu \longrightarrow I + Cl$	1	[1]		Seery and Britton (1964)
Hx 17	$IBr + h\nu \longrightarrow I + Br$	1	[1]		Seery and Britton (1964)

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 CH_3OOH; C_2H_4 is used as generic alkene as in the Lurmann et al. (1986) mechanism. The rate coefficients are calculated with $k = A \times \exp(\frac{-E_a}{RT})$.

Table 3: Aqueous phase reactions.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
O 1	$O_3 + OH \longrightarrow HO_2$	2	1.1 x 10^8		Sehested et al. (1984)
O 2	$O_3 + O_2^- \longrightarrow OH + OH^-$	2	1.5 x 10^9		Sehested et al. (1983)
O 3	$OH + OH \longrightarrow H_2O_2$	2	5.5 x 10^9		Buxton et al. (1988)
O 4	$OH + HO_2 \longrightarrow H_2O$	2	7.1 x 10^9		Sehested et al. (1968)
O 5	$OH + O_2^- \longrightarrow OH^-$	2	1.0 x 10^{10}		Sehested et al. (1968)
O 6	$OH + H_2O_2 \longrightarrow HO_2$	2	2.7 x 10^7	-1684	Christensen et al. (1982)
O 7	$HO_2 + HO_2 \longrightarrow H_2O_2$	2	9.7 x 10^5	-2500	Christensen and Sehested (1988)
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	1.0 x 10^8	-900	Christensen and Sehested (1988)
N 1	$HONO + OH \longrightarrow NO_2$	2	1.0 x 10^{10}		assumed =N7 Barker et al. (1970)
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3$	3	4.6 x 10^3	-6800	Damschen and Martin (1983)
N 3	$NO_3 + OH^- \longrightarrow NO_3^- + OH$	2	8.2 x 10^7	-2700	Exner et al. (1992)
N 4	$NO_2 + NO_2 \longrightarrow HNO_3 + HONO$	2	1.0 x 10^8		Lee and Schwartz (1981)
N 5	$NO_2 + HO_2 \longrightarrow HNO_4$	2	1.8 x 10^9		Warneck (1999)
N 6	$NO_2^- + O_3 \longrightarrow NO_3^- + O_2$	2	5.0 x 10^5	-6950	Damschen and Martin (1983)
N 7	$NO_2^- + OH \longrightarrow NO_2 + OH^-$	2	1.0 x 10^{10}		Barker et al. (1970)
N 8	$NO_4^- \longrightarrow NO_2^- + O_2$	1	8.0 x 10^{-1}		Warneck (1999)
C 1	$HCHO + OH \longrightarrow HCOOH + HO_2$	2	7.7 x 10^8	-1020	Chin and Wine (1994)
C 2	$HCOOH + OH \longrightarrow HO_2 + CO_2$	2	1.1 x 10^8	-991	Chin and Wine (1994)
C 3	$HCOO^- + OH \longrightarrow OH^- + HO_2 + CO_2$	2	3.1 x 10^9	-1240	Chin and Wine (1994)
C 4	$CH3OO + HO_2 \longrightarrow CH_3OOH$	2	4.3 x 10^5		estimated by Jacob (1986)
C 5	$CH3OO + O_2^- \longrightarrow CH_3OOH + OH^-$	2	5.0 x 10^7		estimated by Jacob (1986)
C 6	$CH_3OH + OH \longrightarrow HCHO + HO_2$	2	9.7 x 10^8		Buxton et al. (1988)
C 7	$CH_3OOH + OH \longrightarrow CH3OO$	2	2.7 x 10^7	-1715	estimated by Jacob (1986)
C 8	$CH_3OOH + OH \longrightarrow HCHO + OH$	2	1.1 x 10^7	-1715	estimated by Jacob (1986)
C 9	$CO_3^- + O_2^- \longrightarrow HCO_3^- + OH^-$	2	6.5 x 10^8		Ross et al. (1992)
C 10	$CO_3^- + H_2O_2 \longrightarrow HCO_3^- + HO_2$	2	4.3 x 10^5		Ross et al. (1992)
C 11	$CO_3^- + HCOO^- \longrightarrow HCO_3^- + HCO_3^- + HO_2$	2	1.5 x 10^5		Ross et al. (1992)
C 12	$HCO_3^- + OH \longrightarrow CO_3^-$	2	8.5 x 10^6		Ross et al. (1992)
C 13	$DOM + OH \longrightarrow HO_2$	2	5.0 x 10^9		estimated by Anastasio et al. (2003) from Ross et al. (1998)
S 1	$SO_3^- + O_2 \longrightarrow SO_5^-$	2	1.5 x 10^9		Huie and Neta (1987)
S 2	$HSO_3^- + O_3 \longrightarrow SO_4^{2-} + H^+ + O_2$	2	3.7 x 10^5	-5500	Hoffmann (1986)
S 3	$SO_3^{2-} + O_3 \longrightarrow SO_4^{2-} + O_2$	2	1.5 x 10^9	-5300	Hoffmann (1986)
S 4	$HSO_3^- + OH \longrightarrow SO_3^-$	2	4.5 x 10^9		Buxton et al. (1988)
S 5	$SO_3^{2-} + OH \longrightarrow SO_3^- + OH^-$	2	5.5 x 10^9		Buxton et al. (1988)
S 6	$HSO_3^- + HO_2 \longrightarrow SO_4^{2-} + OH + H^+$	2	3.0 x 10^3		upper limit D. Sedlak pers. comm. with R. Sander
S 7	$HSO_3^- + O_2^- \longrightarrow SO_4^{2-} + OH$	2	3.0 x 10^3		upper limit D. Sedlak pers. comm. with R. Sander

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
S 8	$HSO_3^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+$	2	$5.2 \times 10^6 \times \frac{[H^+]}{[H^+]+0.1M}$	-3650	Damschen and Martin (1983)
S 9	$HSO_3^- + NO_2 \xrightarrow{NO_2} HSO_4^- + HONO + HONO$	2	2.0 x 10^7		Clifton et al. (1988)
S 10	$SO_3^{2-} + NO_2 \xrightarrow{NO_2} SO_4^{2-} + HONO + HONO$	2	2.0 x 10^7		Clifton et al. (1988)
S 11	$HSO_3^- + NO_3 \longrightarrow SO_3^- + NO_3^- + H^+$	2	1.4 x 10^9	-2000	Exner et al. (1992)
S 12	$HSO_3^- + HNO_4 \longrightarrow HSO_4^- + NO_3^- + H^+$	2	3.1 x 10^5		Warneck (1999)
S 13	$HSO_3^- + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + H^+ + CH_3OH$	3	1.6 x 10^7	-3800	Lind et al. (1987)
S 14	$SO_3^{2-} + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + CH_3OH$	3	1.6 x 10^7	-3800	Lind et al. (1987)
S 15	$HSO_3^- + HCHO \longrightarrow CH_2OHSO_3^-$	2	4.3 x 10^{-1}		Boyce and Hoffmann (1984)
S 16	$SO_3^{2-} + HCHO \xrightarrow{H^+} CH_2OHSO_3^-$	2	1.4 x 10^4		Boyce and Hoffmann (1984)
S 17	$CH_2OHSO_3^- + OH^- \longrightarrow SO_3^{2-} + HCHO$	2	3.6 x 10^3		Seinfeld and Pandis (1998)
S 18	$HSO_3^- + HSO_5^- \xrightarrow{H^+} SO_4^{2-} + SO_4^{2-} + H^+ + H^+$	3	7.1 x 10^6		Betterton and Hoffmann (1988)
S 19	$SO_4^- + OH \longrightarrow HSO_5^-$	2	1.0 x 10^9		Jiang et al. (1992)
S 20	$SO_4^- + HO_2 \longrightarrow SO_4^{2-} + H^+$	2	3.5 x 10^9		Jiang et al. (1992)
S 21	$SO_4^- + O_2^- \longrightarrow SO_4^{2-}$	2	3.5 x 10^9		assumed =S20
S 22	$SO_4^- + H_2O \longrightarrow SO_4^{2-} + H^+ + OH$	2	1.1 x 10^1	-1110	Herrmann et al. (1995)
S 23	$SO_4^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+ + HO_2$	2	1.2 x 10^7		Wine et al. (1989)
S 24	$SO_4^- + NO_3^- \longrightarrow SO_4^{2-} + NO_3$	2	5.0 x 10^4		Exner et al. (1992)
S 25	$SO_4^- + HSO_3^- \longrightarrow SO_3^- + SO_4^{2-} + H^+$	2	8.0 x 10^8		Huie and Neta (1987)
S 26	$SO_4^- + SO_3^{2-} \longrightarrow SO_3^- + SO_4^{2-}$	2	4.6 x 10^8		Huie and Neta (1987)
S 27	$SO_4^{2-} + NO_3 \longrightarrow NO_3^- + SO_4^-$	2	1.0 x 10^5		Logager et al. (1993)
S 28	$SO_5^- + HSO_3^- \longrightarrow SO_4^- + SO_4^{2-} + H^+$	2	7.5 x 10^4		Huie and Neta (1987)
S 29	$SO_5^- + SO_3^{2-} \longrightarrow SO_4^- + SO_4^{2-}$	2	9.4 x 10^6		Huie and Neta (1987)
S 30	$SO_5^- + HSO_3^- \longrightarrow SO_3^- + HSO_5^-$	2	2.5 x 10^4		Huie and Neta (1987); Deister and Warneck (1990)
S 31	$SO_5^- + SO_3^{2-} \xrightarrow{H^+} SO_3^- + HSO_5^-$	2	3.6 x 10^6		Huie and Neta (1987); Deister and Warneck (1990)
S 32	$SO_5^- + O_2^- \xrightarrow{H^+} HSO_5^- + O_2$	2	2.3 x 10^8		Buxton et al. (1996)
S 33	$SO_5^- + SO_5^- \longrightarrow H_2O$	2	1.0 x 10^8		Ross et al. (1992)
S 34	$DMS + O_3 \longrightarrow O_2 + DMSO$	2	8.6 x 10^8	-2600	Gershenzon et al. (2001)
S 35	$DMS + OH \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH3OO + 0.5\ HSO_4^- + HCHO + H^+$	2	1.9 x 10^{10}		Ross et al. (1998)
S 36	$DMSO + OH \longrightarrow CH_3SO_2^- + CH3OO + H^+$	2	4.5 x 10^9		Bardouki et al. (2002)
S 37	$CH_3SO_2^- + OH \longrightarrow CH_3SO_3^- + H2O - O2$	2	1.2 x 10^{10}		Bardouki et al. (2002)
S 38	$CH_3SO_3^- + OH \longrightarrow SO_4^{2-} + H^+ + CH3OO$	2	1.2 x 10^7		Bonsang et al. (1991)

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
Cl 1	$Cl + H_2O_2 \longrightarrow HO_2 + Cl^- + H^+$	2	2.0 x 10^9		Yu (2001)
Cl 2	$Cl + H_2O \longrightarrow H^+ + ClOH^-$	2	1.8 x 10^5		Yu (2001)
Cl 3	$Cl + NO_3^- \longrightarrow NO_3 + Cl^-$	2	1.0 x 10^8		Buxton et al. (1999b)
Cl 4	$Cl + DOM \longrightarrow Cl^- + HO_2$	2	5.0 x 10^9		estimated by Anastasio et al. (2003) from Ross et al. (1998)
Cl 5	$Cl + SO_4^{2-} \longrightarrow SO_4^- + Cl^-$	2	2.1 x 10^8		Buxton et al. (1999a)
Cl 6	$Cl + Cl \longrightarrow Cl_2$	2	8.8 x 10^7		Wu et al. (1980)
Cl 7	$Cl^- + OH \longrightarrow ClOH^-$	2	4.2 x 10^9		Yu (2001)
Cl 8	$Cl^- + O_3 \longrightarrow ClO^- + O_2$	2	3.0 x 10^{-3}		Hoigné et al. (1985)
Cl 9	$Cl^- + NO_3 \longrightarrow NO_3^- + Cl$	2	9.3 x 10^6	-4330	Exner et al. (1992)
Cl 10	$Cl^- + SO_4^- \longrightarrow SO_4^{2-} + Cl$	2	2.5 x 10^8		Buxton et al. (1999a)
Cl 11	$Cl^- + HSO_5^- \longrightarrow HOCl + SO_4^{2-}$	2	1.8 x 10^{-3}	-7352	Fortnum et al. (1960)
Cl 12	$Cl^- + HOCl + H^+ \longrightarrow Cl_2$	3	2.2 x 10^4	-3508	Ayers et al. (1996)
Cl 13	$Cl_2 \longrightarrow Cl^- + HOCl + H^+$	1	2.2 x 10^1	-8012	Ayers et al. (1996)
Cl 14	$Cl_2^- + OH \longrightarrow HOCl + Cl^-$	2	1.0 x 10^9		Ross et al. (1998)
Cl 15	$Cl_2^- + OH^- \longrightarrow Cl^- + Cl^- + OH$	2	4.0 x 10^6		Jacobi (1996)
Cl 16	$Cl_2^- + HO_2 \longrightarrow Cl^- + Cl^- + H^+ + O_2$	2	3.1 x 10^9		Yu (2001)
Cl 17	$Cl_2^- + O_2^- \longrightarrow Cl^- + Cl^- + O_2$	2	6.0 x 10^9		Jacobi (1996)
Cl 18	$Cl_2^- + H_2O_2 \longrightarrow Cl^- + Cl^- + H^+ + HO_2$	2	7.0 x 10^5	-3340	Jacobi (1996)
Cl 19	$Cl_2^- + NO_2^- \longrightarrow Cl^- + Cl^- + NO_2$	2	6.0 x 10^7		Jacobi (1996)
Cl 20	$Cl_2^- + CH_3OOH \longrightarrow Cl^- + Cl^- + H^+ + CH3OO$	2	7.0 x 10^5	-3340	assumed by Jacobi (1996)
Cl 21	$Cl_2^- + DOM \longrightarrow Cl^- + Cl^- + HO_2$	2	1.0 x 10^6		estimated by Anastasio et al. (2003) from Ross et al. (1998)
Cl 22	$Cl_2^- + HSO_3^- \longrightarrow SO_3^- + Cl^- + Cl^- + H^+$	2	4.7 x 10^8	-1082	Shoute et al. (1991)
Cl 23	$Cl_2^- + SO_3^{2-} \longrightarrow SO_3^- + Cl^- + Cl^-$	2	6.2 x 10^7		Jacobi et al. (1996)
Cl 24	$Cl_2^- + Cl_2^- \longrightarrow Cl_2 + 2Cl^-$	2	6.2 x 10^9		Yu (2001)
Cl 25	$Cl_2^- + Cl \longrightarrow Cl^- + Cl_2$	2	2.7 x 10^9		Yu (2001)
Cl 26	$Cl_2^- + DMS \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH3OO + 0.5\ HSO_4^- + HCHO + 2\ Cl^- + 2\ H^+$	2	3.0 x 10^9		rate from Ross et al. (1998)
Cl 27	$ClOH^- \longrightarrow Cl^- + OH$	1	6.0 x 10^9		Yu (2001)
Cl 28	$ClOH^- + H^+ \longrightarrow Cl$	2	4.0 x 10^{10}		Yu (2001)
Cl 29	$HOCl + HO_2 \longrightarrow Cl + O_2$	2	7.5 x 10^6		assumed = Cl30 Long and Bielski (1980)
Cl 30	$HOCl + O_2^- \longrightarrow Cl + OH^- + O_2$	2	7.5 x 10^6		Long and Bielski (1980)
Cl 31	$HOCl + SO_3^{2-} \longrightarrow Cl^- + HSO_4^-$	2	7.6 x 10^8		Fogelman et al. (1989)
Cl 32	$HOCl + HSO_3^- \longrightarrow Cl^- + HSO_4^- + H^+$	2	7.6 x 10^8		assumed = Cl31 Fogelman et al. (1989)
Cl 33	$Cl_2 + HO_2 \longrightarrow Cl_2^- + H^+ + O_2$	2	1.0 x 10^9		Bjergbakke et al. (1981)
Cl 34	$Cl_2 + O_2^- \longrightarrow Cl_2^- + O_2$	2	1.0 x 10^9		assumed = Cl33 Bjergbakke et al. (1981)

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
Br 1	$Br + OH^- \longrightarrow BrOH^-$	2	1.3 x 10^{10}		Zehavi and Rabani (1972)
Br 2	$Br + DOM \longrightarrow Br^- + HO_2$	2	2.0 x 10^8		estimated by Anastasio et al. (2003) from Ross et al. (1998)
Br 3	$Br^- + OH \longrightarrow BrOH^-$	2	1.1 x 10^{10}		Zehavi and Rabani (1972)
Br 4	$Br^- + O_3 \longrightarrow BrO^-$	2	2.1 x 10^2	-4450	Haag and Hoigné (1983)
Br 5	$Br^- + NO_3 \longrightarrow Br + NO_3^-$	2	3.8 x 10^9		Zellner et al. 1996 in Herrmann et al. (2000)
Br 6	$Br^- + SO_4^- \longrightarrow Br + SO_4^{2-}$	2	2.1 x 10^9		Jacobi (1996)
Br 7	$Br^- + HSO_5^- \longrightarrow HOBr + SO_4^{2-}$	2	1.0	-5338	Fortnum et al. (1960)
Br 8	$Br^- + HOBr + H^+ \longrightarrow Br_2$	3	1.6 x 10^{10}		Liu and Margerum (2001)
Br 9	$Br_2 \longrightarrow Br^- + HOBr + H^+$	1	9.7 x 10^1	7457	Liu and Margerum (2001)
Br 10	$Br_2^- + O_2^- \longrightarrow Br^- + Br^-$	2	1.7 x 10^8		Wagner and Strehlow (1987)
Br 11	$Br_2^- + HO_2 \longrightarrow Br_2 + H_2O_2$ - H^+	2	4.4 x 10^9		Matthew et al. (2003)
Br 12	$Br_2^- + H_2O_2 \longrightarrow Br^- + Br^- + H^+ + HO_2$	2	5.0 x 10^2		Chameides and Stelson (1992)
Br 13	$Br_2^- + Br_2^- \longrightarrow Br^- + Br^- + Br_2$	2	1.9 x 10^9		Ross et al. (1992)
Br 14	$Br_2^- + CH_3OOH \longrightarrow Br^- + Br^- + H^+ +$ CH3OO	2	1.0 x 10^5		assumed by Jacobi (1996)
Br 15	$Br_2^- + DOM \longrightarrow Br^- + Br^- + HO_2$	2	1.0 x 10^5		estimated by Anastasio et al. (2003) from Ross et al. (1998)
Br 16	$Br_2^- + NO_2^- \longrightarrow Br^- + Br^- + NO_2$	2	1.7 x 10^7	-1720	Shoute et al. (1991)
Br 17	$Br_2^- + HSO_3^- \longrightarrow Br^- + Br^- + H^+ + SO_3^-$	2	6.3 x 10^7	-782	Shoute et al. (1991)
Br 18	$Br_2^- + SO_3^{2-} \longrightarrow Br^- + Br^- + SO_3^-$	2	2.2 x 10^8	-650	Shoute et al. (1991)
Br 19	$Br_2^- + DMS \longrightarrow 0.5\ CH_3SO_3^- +$ 0.5 CH3OO $+ 0.5\ HSO_4^- + HCHO + 2\ Br^- + 2\ H^+$	2	3.2 x 10^9		rate from Ross et al. (1998)
Br 20	$BrOH^- \longrightarrow Br^- + OH$	1	3.3 x 10^7		Zehavi and Rabani (1972)
Br 21	$BrOH^- \longrightarrow Br + OH^-$	1	4.2 x 10^6		Zehavi and Rabani (1972)
Br 22	$BrOH^- + H^+ \longrightarrow Br$	2	4.4 x 10^{10}		Zehavi and Rabani (1972)
Br 23	$BrOH^- + Br^- \longrightarrow Br_2^- + OH^-$	2	1.9 x 10^8		Zehavi and Rabani (1972)
Br 24	$BrO^- + SO_3^{2-} \longrightarrow Br^- + SO_4^{2-}$	2	1.0 x 10^8		Troy and Margerum (1991)
Br 25	$HOBr + HO_2 \longrightarrow Br + O_2$	2	1.0 x 10^9		Herrmann et al. (1999)
Br 26	$HOBr + O_2^- \longrightarrow Br + OH^- + O_2$	2	3.5 x 10^9		Schwarz and Bielski (1986)
Br 27	$HOBr + H_2O_2 \longrightarrow Br^- + H^+ + O_2$	2	1.2 x 10^6		von Gunten and Oliveras (1998)
Br 28	$HOBr + SO_3^{2-} \longrightarrow Br^- + HSO_4^-$	2	5.0 x 10^9		Troy and Margerum (1991)
Br 29	$HOBr + HSO_3^- \longrightarrow Br^- + HSO_4^- + H^+$	2	5.0 x 10^9		assumed = Br28
Br 30	$Br_2 + HO_2 \longrightarrow Br_2^- + H^+ + O_2$	2	1.1 x 10^8		Ross et al. (1998)
Br 31	$Br_2 + O_2^- \longrightarrow Br_2^- + O_2$	2	5.6 x 10^9		Ross et al. (1998)

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
I 1	$HOI + I^- + H^+ \longrightarrow I_2$	3	4.4×10^{12}		Eigen and Kustin (1962)
I 2	$HOI + Cl^- + H^+ \longrightarrow ICl$	3	2.9×10^{10}		Wang et al. (1989)
I 3	$ICl \longrightarrow HOI + Cl^- + H^+$	1	2.4×10^{6}		Wang et al. (1989)
I 4	$HOI + Br^- + H^+ \longrightarrow IBr$	3	3.3×10^{12}		Troy et al. (1991)
I 5	$IBr \longrightarrow HOI + H^+ + Br^-$	1	8.0×10^{5}		Troy et al. (1991)
I 6	$HOCl + I^- + H^+ \longrightarrow ICl$	3	3.5×10^{11}		Nagy et al. (1988)
I 7	$HOBr + I^- \longrightarrow IBr + OH^-$	2	5.0×10^{9}		Troy and Margerum (1991)
I 9	$IO_2^- + H_2O_2 \longrightarrow IO_3^-$	2	6.0×10^{1}		Furrow (1987)
I 10	$IO + IO \longrightarrow HOI + IO_2^- + H^+$	2	1.5×10^{9}		Buxton et al. (1986)
I 11	$I^- + O_3 \xrightarrow{H^+} HOI$	2	4.2×10^{9}	-9311	Magi et al. (1997)
I 12	$HOI + Cl_2 \longrightarrow IO_2^- + 2Cl^- + 3H^+$	2	1.0×10^{6}		Lengyel et al. (1996)
I 13	$HOI + HOCl \longrightarrow IO_2^- + Cl^- + 2\ H^+$	2	5.0×10^{5}		Citri and Epstein (1988)
I 14	$HOI + HOBr \longrightarrow IO_2^- + Br^- + 2\ H^+$	2	1.0×10^{6}		Chinake and Simoyi (1996)
I 15	$IO_2^- + HOCl \longrightarrow IO_3^- + Cl^- + H^+$	2	1.5×10^{3}		Lengyel et al. (1996)
I 16	$IO_2^- + HOBr \longrightarrow IO_3^- + Br^- + H^+$	2	1.0×10^{6}		Chinake and Simoyi (1996)
I 17	$IO_2^- + HOI \longrightarrow IO_3^- + I^- + H^+$	2	6.0×10^{2}		Chinake and Simoyi (1996)
I 18	$I_2 + HSO_3^- \longrightarrow 2\ I^- + HSO_4^- + 2\ H^+$	2	1.0×10^{6}		Olsen and Epstein (1991)
Hx 1	$Br^- + HOCl + H^+ \longrightarrow BrCl$	3	$1.3 \text{ x } 10^{6}$		Liu and Margerum (2001)
Hx 2	$Cl^- + HOBr + H^+ \longrightarrow BrCl$	3	$2.3 \text{ x } 10^{10}$		Liu and Margerum (2001)
Hx 3	$BrCl \longrightarrow Cl^- + HOBr + H^+$	1	$3.0 \text{ x } 10^{6}$		Liu and Margerum (2001)
Hx 4	$Br^- + ClO^- + H^+ \longrightarrow BrCl + OH^-$	3	$3.7 \text{ x } 10^{10}$		Kumar and Margerum (1987)
Hx 5	$Cl_2 + Br^- \longrightarrow BrCl_2^-$	2	$7.7 \text{ x } 10^{9}$		Liu and Margerum (2001)
Hx 6	$BrCl_2^- \longrightarrow Cl_2 + Br^-$	1	$1.83 \text{ x } 10^{3}$		Liu and Margerum (2001)
hv 1	$O_3 + hv \longrightarrow OH + OH + O_2$	[1]	1		assumed 2x gas phase
hv 2	$H_2O_2 + hv \longrightarrow OH + OH$	[1]	1		assumed 2x gas phase
hv 3	$NO_3^- + hv \xrightarrow{H^+} NO_2 + OH$	[1]	1		Zellner et al. (1990)
hv 4	$NO_2^- + hv \xrightarrow{H^+} NO + OH$	[1]	1		Zellner et al. (1990); Burley and Johnston (1992)
hv 5	$HOCl + hv \longrightarrow OH + Cl$	[1]	1		assumed 2x gas phase
hv 6	$Cl_2 + hv \longrightarrow Cl + Cl$	[1]	1		assumed 2x gas phase
hv 7	$HOBr + hv \longrightarrow OH + Br$	[1]	1		assumed 2x gas phase
hv 8	$Br_2 + hv \longrightarrow Br + Br$	[1]	1		assumed 2x gas phase
hv 9	$BrCl + hv \longrightarrow Cl + Br$	[1]	1		assumed 2x gas phase

n is the order of the reaction. [1] photolysis rates calculated online. The temperature dependence is $k = k_0 \times \exp(\frac{-E_a}{R}(\frac{1}{T} - \frac{1}{T_0}))$, $T_0 = 298$ K.

Table 4: Heterogeneous reactions.

no	reaction	k	reference
H 1	$N_2O_5 \xrightarrow{H_2O} HNO_{3aq} + HNO_{3aq}$	$\overline{k_t}(N_2O_5)w_{l,i}[H_2O]/Het_T$	Behnke et al. (1994), Behnke et al. (1997)
H 2	$N_2O_5 \xrightarrow{Cl^-} ClNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	Behnke et al. (1994), Behnke et al. (1997)
H 3	$N_2O_5 \xrightarrow{Br^-} BrNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Br^-)[Br^-]/Het_T$	Behnke et al. (1994), Behnke et al. (1997)
H 4	$ClNO_3 \xrightarrow{H_2O} HOCl_{aq} + HNO_{3aq}$	$\overline{k_t}(ClNO_3)w_{l,i}[H_2O]/Het_T$	see note
H 5	$ClNO_3 \xrightarrow{Cl^-} Cl_{2aq} + NO_3^-$	$\overline{k_t}(ClNO_3)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	see note
H 6	$ClNO_3 \xrightarrow{Br^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(ClNO_3)w_{l,i}f(Br^-)[Br^-]/Het_T$	see note
H 7	$BrNO_3 \xrightarrow{H_2O} HOBr_{aq} + HNO_{3aq}$	$\overline{k_t}(BrNO_3)w_{l,i}[H_2O]/Het_T$	see note
H 8	$BrNO_3 \xrightarrow{Cl^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(BrNO_3)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	see note
H 9	$BrNO_3 \xrightarrow{Br^-} Br_{2aq} + NO_3^-$	$\overline{k_t}(BrNO_3)w_{l,i}f(Br^-)[Br^-]/Het_T$	see note
H 10	$INO_3 \xrightarrow{H_2O} HOI_{aq} + HNO_{3aq}$	$\overline{k_t}(INO_3)w_{l,i}$	
H 11	$HI \xrightarrow{H_2O} H^+ + I^-$	$\overline{k_t}(HI)w_{l,i}$	
H 12	$INO_2 \xrightarrow{H_2O} HOI_{aq} + HONO_{aq}$	$\overline{k_t}(INO_2)w_{l,i}$	
H 13	$OIO \xrightarrow{H_2O} HOI_{aq} + HO_{2aq}$	$\overline{k_t}(OIO)w_{l,i}$	assumed, see von Glasow et al. (2002b)
H 14	$HIO_3 \xrightarrow{H_2O} IO_3^- + H^+$	$\overline{k_t}(HIO_3)w_{l,i}$	assumed, see von Glasow et al. (2002b)

For a definition of $\overline{k_t}$ and $w_{l,i}$ see von Glasow et al. (2002a) or von Glasow (2000). $Het_T = [H_2O + f(Cl^-)[Cl^-] + f(Br^-)[Br^-]$, with $f(Cl^-) = 5.0 \times 10^2$ and $f(Br^-) = 3.0 \times 10^5$. H4 - H9: the total rate is determined by $\overline{k_t}$, the distribution among the different reaction paths was assumed to be the same as for reactions H1 - H3.

Table 5: Aqueous phase equilibrium constants.

no	reaction	m	n	K_0 [M^{n-m}]	-$\Delta H/R$ [K]	reference
EQ 1	$CO_{2aq} \longleftrightarrow H^+ + HCO_3^-$	1	2	4.3×10^{-7}	-913	Chameides (1984)
EQ 2	$NH_{3aq} \longleftrightarrow OH^- + NH_4^+$	1	2	1.7×10^{-5}	-4325	Chameides (1984)
EQ 3	$H_2O_{aq} \longleftrightarrow H^+ + OH^-$	1	2	1.0×10^{-14}	-6716	Chameides (1984)
EQ 4	$HCOOH_{aq} \longleftrightarrow H^+ + HCOO^-$	1	2	1.8×10^{-4}		Weast (1980)
EQ 5	$HSO_3^- \longleftrightarrow H^+ + SO_3^{2-}$	1	2	6.0×10^{-8}	1120	Chameides (1984)
EQ 6	$H_2SO_{4aq} \longleftrightarrow H^+ + HSO_4^-$	1	2	1.0×10^{3}		Seinfeld and Pandis (1998)
EQ 7	$HSO_4^- \longleftrightarrow H^+ + SO_4^{2-}$	1	2	1.2×10^{-2}	1120	Weast (1980)
EQ 8	$HO_{2aq} \longleftrightarrow O_2^- + H^+$	1	2	1.6×10^{-5}		Weinstein-Lloyd and Schwartz (1991)
EQ 9	$SO_{2aq} \longleftrightarrow H^+ + HSO_3^-$	1	2	1.7×10^{-2}	2090	Chameides (1984)
EQ 10	$Cl_2^- \longleftrightarrow Cl_{aq} + Cl^-$	1	2	5.2×10^{-6}		Jayson et al. (1973)
EQ 11	$HOCl_{aq} \longleftrightarrow H^+ + ClO^-$	1	2	3.2×10^{-8}		Lax (1969)
EQ 12	$HBr_{aq} \longleftrightarrow H^+ + Br^-$	1	2	1.0×10^{9}		Lax (1969)
EQ 13	$Br_2^- \longleftrightarrow Br_{aq} + Br^-$	1	2	9.1×10^{-6}		Mamou et al. (1977)
EQ 14	$HOBr_{aq} \longleftrightarrow H^+ + BrO^-$	1	2	2.3×10^{-9}	-3091	Kelley and Tartar (1956)
EQ 15	$BrCl_{aq} + Cl^- \longleftrightarrow BrCl_2^-$	2	1	3.8	1143	Wang et al. (1994)
EQ 16	$BrCl_{aq} + Br^- \longleftrightarrow Br_2Cl^-$	2	1	1.8×10^{4}		Wang et al. (1994)
EQ 17	$Br_{2aq} + Cl^- \longleftrightarrow Br_2Cl^-$	2	1	1.3		Wang et al. (1994)
EQ 18	$HNO_{3aq} \longleftrightarrow H^+ + NO_3^-$	1	2	1.5×10^{1}		Davis and de Bruin (1964)
EQ 19	$HCl_{aq} \longleftrightarrow H^+ + Cl^-$	1	2	1.7×10^{6}		Marsh and McElroy (1985)
EQ 20	$HONO_{aq} \longleftrightarrow H^+ + NO_2^-$	1	2	5.1×10^{-4}	-1260	Schwartz and White (1981)
EQ 21	$HNO_{4aq} \longleftrightarrow NO_4^- + H^+$	1	2	1.0×10^{-5}	8700	Warneck (1999)
EQ 22	$ICl_{aq} + Cl^- \longleftrightarrow ICl_2^-$	2	1	7.7×10^{1}		Wang et al. (1989)
EQ 23	$IBr_{aq} + Br^- \longleftrightarrow IBr_2^-$	2	1	2.9×10^{2}		Troy et al. (1991)
EQ 24	$ICl_{aq} + Br^- \longleftrightarrow IClBr^-$	2	1	1.8×10^{4}		assumed = EQ 16
EQ 25	$IBr_{aq} + Cl^- \longleftrightarrow IClBr^-$	2	1	1.3		assumed = EQ 17

The temperature dependence is $K = K_0 \times \exp(\frac{-\Delta H}{R}(\frac{1}{T} - \frac{1}{T_0}))$, $T_0 = 298$ K.

Table 6: Henry constants and accommodation coefficients.

specie	K_H^0 [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	α^0	$-\Delta_{obs}H/R$ [K]	reference
O_3	1.2×10^{-2}	2560	Chameides (1984)	0.002	(at 292 K)	DeMore et al. (1997)
O_2	1.3×10^{-3}	1500	Wilhelm et al. (1977)	0.01	2000	estimated
OH	3.0×10^{1}	4300	Hanson et al. (1992)	0.01	(at 293 K)	Takami et al. (1998)
HO_2	3.9×10^{3}	5900	Hanson et al. (1992)	0.2	(at 293 K)	DeMore et al. (1997)
H_2O_2	1.0×10^{5}	6338	Lind and Kok (1994)	0.077	2769	Worsnop et al. (1989)
NO_2	6.4×10^{-3}	2500	Lelieveld and Crutzen (1991)	0.0015	(at 298 K)	Ponche et al. (1993)
NO_3	2.0	2000	Thomas et al. (1993)	0.04	(at 273? K)	Rudich et al. (1996)
N_2O_5	∞	—		0.1	(at 195-300 K)	DeMore et al. (1997)
HONO	4.9×10^{1}	4780	Schwartz and White (1981)	0.04	(at 247-297 K)	DeMore et al. (1997)
HNO_3	1.7×10^{5}	8694	Lelieveld and Crutzen (1991)	0.5	(at RT)	Abbatt and Waschewsky (1998)
HNO_4	1.2×10^{4}	6900	Régimbal and Mozurkewich (1997)	0.1	(at 200 K)	DeMore et al. (1997)
NH_3	5.8×10^{1}	4085	Chameides (1984)	0.06	(at 295 K)	DeMore et al. (1997)
CH3OO	6.0	$=HO_2$	Pandis and Seinfeld (1989)	0.01	2000	estimated
ROOH	3.0×10^{2}	5322	Lind and Kok (1994)	0.0046	3273	Magi et al. (1997)
HCHO	7.0×10^{3}	6425	Chameides (1984)	0.04	(at 260-270 K)	DeMore et al. (1997)
HCOOH	3.7×10^{3}	5700	Chameides (1984)	0.014	3978	DeMore et al. (1997)
CO_2	3.1×10^{-2}	2423	Chameides (1984)	0.01	2000	estimated
HCl	1.2	9001	Brimblecombe and Clegg (1989)	0.074	3072	Schweitzer et al. (2000)
HOCl	6.7×10^{2}	5862	Huthwelker et al. (1995)	=HOBr	=HOBr	estimated
$ClNO_3$	∞	—		0.1	(at RT)	Koch and Rossi (1998)
Cl_2	9.1×10^{-2}	2500	Wilhelm et al. (1977)	0.038	6546	Hu et al. (1995)
HBr	1.3	10239	Brimblecombe and Clegg (1989)	0.031	3940	Schweitzer et al. (2000)
HOBr	9.3×10^{1}	=HOCl	Vogt et al. (1996)	0.5	(at RT)	Abbatt and Waschewsky (1998)
$BrNO_3$	∞	—		0.8	0	Hanson et al. (1996)
Br_2	7.6×10^{-1}	4094	Dean (1992)	0.038	6546	Hu et al. (1995)
BrCl	9.4×10^{-1}	5600	Bartlett and Margerum (1999)	$=Cl_2$	$=Cl_2$	estimated
DMSO	5.0×10^{4}	=HCHO	De Bruyn et al. (1994)	0.048	2578	De Bruyn et al. (1994)
$DMSO_2$	∞	—	assumed	0.03	5388	De Bruyn et al. (1994)
SO_2	1.2	3120	Chameides (1984)	0.11	0	DeMore et al. (1997)
H_2SO_4	∞	—		0.65	(at 303 K)	Pöschl et al. (1998)
CH_3SO_2H	∞	—	assumed	0.0002	0	Lucas and Prinn (2002)
CH_3SO_3H	∞	—	assumed	0.076	1762	De Bruyn et al. (1994)

Table 7: Henry constants and accommodation coefficients.

specie	K_H^0 [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	α^0	$-\Delta_{obs}H/R$ [K]	reference
HI	∞	—		0.036	4130	Schweitzer et al. (2000)
IO	4.5×10^2	=HOI	estimated by Vogt et al. (1999)	0.5	2000	estimated by Vogt et al. (1999)
HOI	4.5×10^2	=HOCl	Chatfield and Crutzen (1990)	=HOBr	=HOBr	estimated
INO_2	∞	—		0.1	2000	estimated by Vogt et al. (1999)
INO_3	∞	—		0.1	2000	estimated by Vogt et al. (1999)
I_2	3.0	4431	Palmer et al. (1985)	0.01	2000	estimated by Vogt et al. (1999)
ICl	1.1×10^2	=BrCl	Wagman et al. (1982)	0.01	2000	estimated by Vogt et al. (1999)
IBr	2.4×10^1	=BrCl	Wagman et al. (1982)	0.01	2000	estimated by Vogt et al. (1999)
OIO	∞	—		1		estimated
HIO_3	∞	—		0.01	2000	estimated

For ROOH the values of CH_3OOH have been assumed. The temperature dependence is for the Henry constants is $K_H = K_H^0 \times \exp(\frac{-\Delta_{soln}H}{R}(\frac{1}{T} - \frac{1}{T_0}))$, $T_0 = 298$ K and for the accommodation coefficients $dln(\frac{\alpha}{1-\alpha})/d(\frac{1}{T}) = \frac{-\Delta_{obs}H}{R}$. RT stands for "room temperature".

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