Kinetic data for MISTRA-MPIC

supplemental material to:

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Model study of multiphase DMS
oxidation with a focus on halogens

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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 6).

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
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
SO_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
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
Cl, HCl, HOCl, Cl_2
Br, HBr, HOBr, Br_2, BrCl
SO_2, H_2SO_4, DMSO, $DMSO_2$, CH_3SO_2H, CH_3SO_3H
Liquid phase (ions)
H^+, OH^-, O_2^-
NO_2^-, NO_3^-, NO_4^-, NH_4^+
HCO_3^-, CO_3^-, $HCOO^-$
Cl^-, Cl_2^-, ClO^-, $ClOH^-$
Br^-, Br_2^-, BrO^-, $BrCl_2^-$, Br_2Cl^-, $BrOH^-$
HSO_3^-, $SO_3{}^2-$, HSO_4^-, SO_4^{2-}, HSO_5^-, SO_3^-, SO_4^-, SO_5^-, $CH_3SO_3^-$, $CH_2OHSO_2^-$, $CH_2OHSO_3^-$

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	*DeMore et al.* (1997)
O 2	$O^1D + N_2 \longrightarrow O_3$	2	1.8×10^{-11}	110	*DeMore et al.* (1997)
O 3	$O^1D + H_2O \longrightarrow 2\ OH$	2	2.2×10^{-10}		*DeMore et al.* (1997)
O 4	$O_3 + OH \longrightarrow HO_2 + O_2$	2	1.5×10^{-12}	-880	*Sander et al.* (2000)
O 5	$O_3 + HO_2 \longrightarrow OH + 2O_2$	2	2.0×10^{-14}	-680	*Sander et al.* (2000)
O 6	$O_3 + h\nu \longrightarrow O_2 + O^1D$	1	[1]		*DeMore et al.* (1997)
O 7	$HO_2 + OH \longrightarrow H_2O + O_2$	2	4.8×10^{-11}	250	*DeMore et al.* (1997)
O 8	$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$	2	[2]		*DeMore et al.* (1997)
O 9	$H_2O_2 + h\nu \longrightarrow 2OH$	1	[1]		*DeMore et al.* (1997)
O 10	$H_2O_2 + OH \longrightarrow HO_2 + H_2O$	2	2.9×10^{-12}	-160	*DeMore et al.* (1997)
N 1	$NO + OH \xrightarrow{M} HONO$	2	[2]		*DeMore et al.* (1997)
N 2	$NO + HO_2 \longrightarrow NO_2 + OH$	2	3.5×10^{-12}	250	*DeMore et al.* (1997)
N 3	$NO + O_3 \longrightarrow NO_2 + O_2$	2	3.0×10^{-12}	-1500	*Sander et al.* (2000)
N 4	$NO + NO_3 \longrightarrow 2NO_2$	2	1.5×10^{-11}	170	*DeMore et al.* (1997)
N 5	$NO_2 + OH \xrightarrow{M} HNO_3$	2	[2]		*Sander et al.* (2000)
N 6	$NO_2 + HO_2 \xrightarrow{M} HNO_4$	2	[2]		*Atkinson et al.* (1997)
N 7	$NO_2 + O_3 \longrightarrow NO_3 + O_2$	2	1.2×10^{-13}	-2450	*DeMore et al.* (1997)
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.* (2000)
N 10	$NO_3 + h\nu \longrightarrow NO + O_2$	1	[1]		*Wayne et al.* (1991)
N 11	$NO_3 + h\nu \longrightarrow NO_2 + O_3$	1	[1]		*Wayne et al.* (1991)
N 12	$NO_3 + HO_2 \longrightarrow 0.3\ HNO_3 + 0.7\ OH + 0.7\ NO_2 + O_2$	2	4.40×10^{-12}		*Atkinson et al.* (Dec. 2002)
N 13	$N_2O_5 \xrightarrow{M} NO_2 + NO_3$	1	[2]		*Sander et al.* (2000)
N 14	$N_2O_5 + H_2O \longrightarrow 2HNO_3$	2	2.6×10^{-22}		*Mentel et al.* (1996)
N 15	$N_2O_5 + h\nu \longrightarrow NO_2 + NO_3$	1	[1]		*DeMore et al.* (1997)
N 16	$HONO + OH \longrightarrow NO_2$	2	1.8×10^{-11}	-390	*DeMore et al.* (1997)
N 17	$HONO + h\nu \longrightarrow NO + OH$	1	[1]		*DeMore et al.* (1997)
N 18	$HNO_3 + h\nu \longrightarrow NO_2 + OH$	1	[1]		*DeMore et al.* (1997)
N 19	$HNO_3 + OH \longrightarrow NO_3 + H_2O$	2	[2]		*Atkinson et al.* (1997)
N 20	$HNO_4 \xrightarrow{M} NO_2 + HO_2$	1	[2]		*Atkinson et al.* (1997)
N 21	$HNO_4 + OH \longrightarrow NO_2 + H_2O + O_2$	2	1.3×10^{-12}	380	*DeMore et al.* (1997)
N 22	$HNO_4 + h\nu \longrightarrow NO_2 + HO_2$	1	[1]		*DeMore et al.* (1997)
N 23	$HNO_4 + h\nu \longrightarrow OH + NO_3$	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]		*DeMore et al.* (1997)
C 2	$CH_4 + OH \xrightarrow{O_2} CH_3OO + H_2O$	2	2.4×10^{-12}	-1710	*Lurmann et al.* (1986)
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)
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)
C 6	$HO_2 + CH_3OO \longrightarrow ROOH + O_2$	2	3.8×10^{-13}	800	*DeMore et al.* (1997)
C 7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	7.5×10^{-13}	700	*DeMore et al.* (1997)
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	*DeMore et al.* (1997)
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	$SO_2 + OH \longrightarrow H_2SO_4 + HO_2$	2	[2]		*Lurmann et al.* (1986)
S 2	$CH_3SCH_3 + OH \longrightarrow CH_3SCH_2OO + H_2O$	2	[2]		*Atkinson et al.* (1997)
S 3	$CH_3SCH_3 + OH \xrightarrow{O_2} CH_3SOCH_3 + HO_2$	2	[2]		*Atkinson et al.* (1997)
S 4	$CH_3SCH_3 + NO_3 \xrightarrow{O_2} CH_3SCH_2OO + HNO_3$	2	1.9×10^{-13}	520	*Atkinson et al.* (1999)
S 5	$CH_3SCH_3 + Cl \xrightarrow{O_2} CH_3SCH_2OO + HCl$	2	3.3×10^{-10}		*Atkinson et al.* (1999)
S 6	$CH_3SCH_3 + Br \xrightarrow{O_2} CH_3SCH_2OO + HBr$	2	9.0×10^{-11}	-2386	*Jefferson et al.* (1994)
S 7	$CH_3SCH_3 + BrO \longrightarrow CH_3SOCH_3 + Br$	2	2.54×10^{-14}	850	*Ingham et al.* (1999)
S 8	$CH_3SCH_2OO + NO \longrightarrow HCHO + CH3S + NO2$	2	4.9×10^{-12}	263	*Urbanski et al.* (1997)
S 9	$CH_3SCH_2OO + CH_3SCH_2OO \xrightarrow{O_2} 2\ HCHO + 2\ CH3S$	2	1.0×10^{-11}		*Urbanski et al.* (1997); *Atkinson et al.* (Dec. 2002)
S 10	$CH_3S + O_3 \longrightarrow CH_3SO + O_2$	2	1.15×10^{-12}	432	*Atkinson et al.* (Dec. 2002)
S 11	$CH_3S + NO_2 \longrightarrow CH_3SO + NO$	2	3.0×10^{-11}	210	*Atkinson et al.* (Dec. 2002)
S 12	$CH_3SO + NO_2 \xrightarrow{O_2} 0.82\ CH_3SO_2 + 0.18\ SO_2 + 0.18\ MO_2 + NO$	2	1.2×10^{-11}		*Atkinson et al.* (Dec. 2002); *Kukui et al.* (2000), product ratios from *van Dingenen et al.* (1994)
S 13	$CH_3SO + O_3 \xrightarrow{O_2} CH_3SO_2$	2	6.0×10^{-13}		*Atkinson et al.* (Dec. 2002)
S 14	$CH_3SO_2 \longrightarrow SO_2 + CH_3OO$	1	1.9×10^{13}	-8661	*Barone et al.* (1995)
S 15	$CH_3SO_2 + NO_2 \longrightarrow CH_3SO_3 + NO$	2	2.2×10^{-12}		*Ray et al.* (1996)
S 16	$CH_3SO_2 + O_3 \longrightarrow CH_3SO_3$	2	$3. \times 10^{-13}$		*Barone et al.* (1995)
S 17	$CH_3SO_3 + HO_2 \longrightarrow CH_3SO_3H$	2	$5. \times 10^{-11}$		*Barone et al.* (1995)
S 18	$CH_3SO_3 \xrightarrow{H_2O,O_2} CH_3OO + H_2SO_4$	1	1.36×10^{14}	-11071	*Barone et al.* (1995)
S 19	$CH_3SOCH_3 + OH \longrightarrow 0.95\ CH_3SO_2H + 0.95\ CH_3OO + 0.05\ DMSO_2$	2	8.7×10^{-11}		*Urbanski et al.* (1998)
S 20	$CH_3SO_2H + OH \longrightarrow 0.95\ CH_3SO_2 + 0.05\ CH_3SO_3H + 0.05\ HO_2 + H_2O$	2	$9. \times 10^{-11}$		*Kukui et al.* (2003) [3]
S 21	$CH_3SO_2H + O_3 \xrightarrow{O_2} CH_3SO_3H$	2	2.0×10^{-18}		*Lucas and Prinn* (2002) [4]
S 22	$CH_3SO_2H + NO_3 \longrightarrow CH_3SO_2 + HNO_3$	2	1.0×10^{-13}		*Yin et al.* (1990)
S 25	$CH_3SCH_3 + OH \xrightarrow{NO,2O_3} CH_3SO_2 + HCHO + NO_2$	2	1.12×10^{-11}	-253	*Atkinson et al.* (1999)

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	2.3×10^{-11}	-200	*Sander et al.* (2000)
Cl 2	$Cl + H_2O_2 \longrightarrow HCl + HO_2$	2	1.1×10^{-11}	-980	*DeMore et al.* (1997)
Cl 3	$Cl + CH_4 \xrightarrow{O_2} HCl + CH_3OO$	2	9.6×10^{-12}	-1360	*Sander et al.* (2000)
Cl 4	$Cl + C_2H_6 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	7.7×10^{-11}	-90	*DeMore et al.* (1997)
Cl 5	$Cl + C_2H_4 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	$1. \times 10^{-10}$		see note
Cl 6	$Cl + HCHO \xrightarrow{O_2} HCl + HO_2 + CO$	2	8.1×10^{-11}	-30	*DeMore et al.* (1997)
Cl 7	$Cl + ROOH \longrightarrow CH_3OO + HCl$	2	5.7×10^{-11}		*Wallington et al.* (1990), see note
Cl 8	$Cl + ClNO_3 \longrightarrow Cl_2 + NO_3$	2	9.6×10^{-12}	140	*Yokelson et al.* (1995)
Cl 9	$ClO + HO_2 \longrightarrow HOCl + O_2$	2	4.8×10^{-13}	700	*DeMore et al.* (1997)
Cl 10	$ClO + NO \longrightarrow Cl + NO_2$	2	6.4×10^{-12}	290	*DeMore et al.* (1997)
Cl 11	$ClO + NO_2 \xrightarrow{M} ClNO_3$	2	[2]		*Sander et al.* (2000)
Cl 12	$ClO + CH_3OO \longrightarrow Cl + HCHO + HO_2$	2	3.3×10^{-12}	-115	*DeMore et al.* (1997)
Cl 13	$ClO + ClO \longrightarrow Cl_2O_2$	2	[2]		*Sander et al.* (2000)
Cl 14	$Cl_2O_2 \longrightarrow ClO + ClO$	1	[2]		*Sander et al.* (2000)
Cl 15	$HCl + OH \longrightarrow H_2O + Cl$	2	2.6×10^{-12}	-350	*DeMore et al.* (1997)
Cl 16	$ClNO_3 \longrightarrow ClO + NO_2$	1	[2]		*Anderson and Fahey* (1990)
Cl 17	$OClO + h\nu \xrightarrow{O_2,O_3} O_3 + ClO$	1	[1]		*DeMore et al.* (1997)
Cl 18	$Cl_2O_2 + h\nu \longrightarrow Cl + Cl + O_2$	1	[1]		*DeMore et al.* (1997)
Cl 19	$Cl_2 + h\nu \longrightarrow 2\ Cl$	1	[1]		*DeMore et al.* (1997)
Cl 20	$HOCl + h\nu \longrightarrow Cl + OH$	1	[1]		*DeMore et al.* (1997)
Cl 21	$ClNO_2 + h\nu \longrightarrow Cl + NO_2$	1	[1]		*DeMore et al.* (1997)
Cl 22	$ClNO_3 + h\nu \longrightarrow Cl + NO_3$	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	*DeMore et al.* (1997)
Br 2	$Br + HO_2 \longrightarrow HBr + O_2$	2	1.5×10^{-11}	-600	*DeMore et al.* (1997)
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	*DeMore et al.* (1997)
Br 5	$Br + ROOH \longrightarrow CH_3OO + HBr$	2	2.66×10^{-12}	-1610	*Mallard et al.* (1993), see note
Br 6	$Br + BrNO_3 \longrightarrow Br_2 + NO_3$	2	4.9×10^{-11}		*Orlando and Tyndall* (1996)
Br 7	$BrO + HO_2 \longrightarrow HOBr + O_2$	2	3.4×10^{-12}	540	*DeMore et al.* (1997)
Br 8	$BrO + CH_3OO \longrightarrow HOBr + HCHO$	2	4.1×10^{-12}		*Aranda et al.* (1997)
Br 9	$BrO + CH_3OO \longrightarrow Br + HCHO + HO_2$	2	1.6×10^{-12}		*Aranda et al.* (1997)
Br 10	$BrO + NO \longrightarrow Br + NO_2$	2	8.8×10^{-12}	260	*DeMore et al.* (1997)
Br 11	$BrO + NO_2 \xrightarrow{M} BrNO_3$	2	[2]		*Sander et al.* (2000)
Br 12	$BrO + BrO \longrightarrow 2\,Br + O_2$	2	2.36×10^{-12}	40	*DeMore et al.* (1997)
Br 13	$BrO + BrO \longrightarrow Br_2 + O_2$	2	2.79×10^{-14}	860	*DeMore et al.* (1997)
Br 14	$HBr + OH \longrightarrow Br + H_2O$	2	1.1×10^{-11}		*DeMore et al.* (1997)
Br 15	$BrNO_3 \longrightarrow BrO + NO_2$	1	[2]		*Orlando and Tyndall* (1996)
Br 16	$BrO + h\nu \xrightarrow{O_2} Br + O_3$	1	[1]		*DeMore et al.* (1997)
Br 17	$Br_2 + h\nu \longrightarrow 2\,Br$	1	[1]		*Hubinger and Nee* (1995)
Br 18	$HOBr + h\nu \longrightarrow Br + OH$	1	[1]		*Ingham et al.* (1999)
Br 19	$BrNO_2 + h\nu \longrightarrow Br + NO_2$	1	[1]		*Scheffler et al.* (1997)
Br 20	$BrNO_3 + h\nu \longrightarrow Br + NO_3$	1	[1]		*DeMore et al.* (1997)
Hx 1	$BrO + ClO \longrightarrow Br + OClO$	2	9.5×10^{-13}	550	*Sander et al.* (2000)
Hx 2	$BrO + ClO \longrightarrow Br + Cl + O_2$	2	2.3×10^{-12}	260	*Sander et al.* (2000)
Hx 3	$BrO + ClO \longrightarrow BrCl + O_2$	2	4.1×10^{-13}	290	*Sander et al.* (2000)
Hx 4	$Br_2 + Cl \longrightarrow BrCl + Br$	2	1.2×10^{-10}		*Mallard et al.* (1993)
Hx 5	$BrCl + Br \longrightarrow Br_2 + Cl$	2	3.3×10^{-15}		*Mallard et al.* (1993)
Hx 6	$Br + Cl_2 \longrightarrow BrCl + Cl$	2	1.1×10^{-15}		*Mallard et al.* (1993)
Hx 7	$BrCl + Cl \longrightarrow Br + Cl_2$	2	1.5×10^{-11}		*Mallard et al.* (1993)
Hx 8	$BrCl + h\nu \longrightarrow Br + Cl$	1	[1]		*DeMore et al.* (1997)

n is the order of the reaction. [1] photolysis rates calculated online, [2] special rate functions (pressure dependent and/or humidity dependent), [3] see text for sensitivity studies, [4] only in "Luc" scenario. Notes: ALD is a generic aldehyde (see *Lurmann et al.* (1986)), the rates for ROOH (reactions C32, C33, Cl7, Br5) were assumed as that of CH_3OOH, in reactions C4 and C5 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	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
O 1	$O_3 + OH \longrightarrow HO_2$	1.1 x 10^8		*Sehested et al.* (1984)
O 2	$O_3 + O_2^- \longrightarrow OH + OH^-$	1.5 x 10^9		*Sehested et al.* (1983)
O 3	$OH + OH \longrightarrow H_2O_2$	5.5 x 10^9		*Buxton et al.* (1988)
O 4	$OH + HO_2 \longrightarrow H_2O$	7.1 x 10^9		*Sehested et al.* (1968)
O 5	$OH + O_2^- \longrightarrow OH^-$	1.0 x 10^{10}		*Sehested et al.* (1968)
O 6	$OH + H_2O_2 \longrightarrow HO_2$	2.7 x 10^7	-1684	*Christensen et al.* (1982)
O 7	$HO_2 + HO_2 \longrightarrow H_2O_2$	9.7 x 10^5	-2500	*Christensen and Sehested* (1988)
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	1.0 x 10^8	-900	*Christensen and Sehested* (1988)
N 1	$HONO + OH \longrightarrow NO_2$	1.0 x 10^{10}		assumed =N7 *Barker et al.* (1970)
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3$	4.6 x 10^3	-6800	*Damschen and Martin* (1983)
N 3	$NO_3 + OH^- \longrightarrow NO_3^- + OH$	8.2 x 10^7	-2700	*Exner et al.* (1992)
N 4	$NO_2 + NO_2 \longrightarrow HNO_3 + HONO$	1.0 x 10^8		*Lee and Schwartz* (1981)
N 5	$NO_2 + HO_2 \longrightarrow HNO_4$	1.8 x 10^9		*Warneck* (1999)
N 6	$NO_2^- + O_3 \longrightarrow NO_3^- + O_2$	5.0 x 10^5	-6950	*Damschen and Martin* (1983)
N 7	$NO_2^- + OH \longrightarrow NO_2 + OH^-$	1.0 x 10^{10}		*Barker et al.* (1970)
N 8	$NO_4^- \longrightarrow NO_2^- + O_2$	8.0 x 10^{-1}		*Warneck* (1999)
C 1	$HCHO + OH \longrightarrow HCOOH + HO_2$	7.7 x 10^8	-1020	*Chin and Wine* (1994)
C 2	$HCOOH + OH \longrightarrow HO_2 + CO_2$	1.1 x 10^8	-991	*Chin and Wine* (1994)
C 3	$HCOO^- + OH \longrightarrow OH^- + HO_2 + CO_2$	3.1 x 10^9	-1240	*Chin and Wine* (1994)
C 4	$CH3OO + HO_2 \longrightarrow CH_3OOH$	4.3 x 10^5		estimated by *Jacob* (1986)
C 5	$CH3OO + O_2^- \longrightarrow CH_3OOH + OH^-$	5.0 x 10^7		estimated by *Jacob* (1986)
C 6	$CH_3OH + OH \longrightarrow HCHO + HO_2$	9.7 x 10^8		*Buxton et al.* (1988)
C 7	$CH_3OOH + OH \longrightarrow CH3OO$	2.7 x 10^7	-1715	estimated by *Jacob* (1986)
C 8	$CH_3OOH + OH \longrightarrow HCHO + OH$	1.1 x 10^7	-1715	estimated by *Jacob* (1986)
C 9	$CO_3^- + O_2^- \longrightarrow HCO_3^- + OH^-$	6.5 x 10^8		*Ross et al.* (1992)
C 10	$CO_3^- + H_2O_2 \longrightarrow HCO_3^- + HO_2$	4.3 x 10^5		*Ross et al.* (1992)
C 11	$CO_3^- + HCOO^- \longrightarrow HCO_3^- + HCO_3^- + HO_2$	1.5 x 10^5		*Ross et al.* (1992)
C 12	$HCO_3^- + OH \longrightarrow CO_3^-$	8.5 x 10^6		*Ross et al.* (1992)
C 13	$DOM + OH \longrightarrow HO_2$	5.0 x 10^9		estimated by *Anastasio et al.* (2003) from *Ross et al.* (1998)
S 1	$SO_3^- + O_2 \longrightarrow SO_5^-$	1.5 x 10^9		*Huie and Neta* (1987)
S 2	$HSO_3^- + O_3 \longrightarrow SO_4^{2-} + H^+ + O_2$	3.7 x 10^5	-5500	*Hoffmann* (1986)
S 3	$SO_3^{2-} + O_3 \longrightarrow SO_4^{2-} + O_2$	1.5 x 10^9	-5300	*Hoffmann* (1986)
S 4	$HSO_3^- + OH \longrightarrow SO_3^-$	4.5 x 10^9		*Buxton et al.* (1988)

Table 3: Continued.

no	reaction	k_0 [(M^{1-n})s^{-1}]	$-E_a$ / R [K]	reference
S 5	$SO_3^{2-} + OH \longrightarrow SO_3^- + OH^-$	5.5 x 10^9		*Buxton et al.* (1988)
S 6	$HSO_3^- + HO_2 \longrightarrow SO_4^{2-} + OH + H^+$	3.0 x 10^3		upper limit D. Sedlak pers. comm. with R. Sander
S 7	$HSO_3^- + O_2^- \longrightarrow SO_4^{2-} + OH$	3.0 x 10^3		upper limit D. Sedlak pers. comm. with R. Sander
S 8	$HSO_3^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+$	$5.2 \times 10^6 \times \frac{[H^+]}{[H^+]+0.1M}$	-3650	*Damschen and Martin* (1983)
S 9	$HSO_3^- + NO_2 \xrightarrow{NO_2} HSO_4^- + HONO + HONO$	2.0 x 10^7		*Clifton et al.* (1988)
S 10	$SO_3^{2-} + NO_2 \xrightarrow{NO_2} SO_4^{2-} + HONO + HONO$	2.0 x 10^7		*Clifton et al.* (1988)
S 11	$HSO_3^- + NO_3 \longrightarrow SO_3^- + NO_3^- + H^+$	1.4 x 10^9	-2000	*Exner et al.* (1992)
S 12	$HSO_3^- + HNO_4 \longrightarrow HSO_4^- + NO_3^- + H^+$	3.1 x 10^5		*Warneck* (1999)
S 13	$HSO_3^- + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + H^+ + CH_3OH$	1.6 x 10^7	-3800	*Lind et al.* (1987)
S 14	$SO_3^{2-} + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + CH_3OH$	1.6 x 10^7	-3800	*Lind et al.* (1987)
S 15	$HSO_3^- + HCHO \longrightarrow CH_2OHSO_3^-$	4.3 x 10^{-1}		*Boyce and Hoffmann* (1984)
S 16	$SO_3^{2-} + HCHO \xrightarrow{H^+} CH_2OHSO_3^-$	1.4 x 10^4		*Boyce and Hoffmann* (1984)
S 17	$CH_2OHSO_3^- + OH^- \longrightarrow SO_3^{2-} + HCHO$	3.6 x 10^3		*Seinfeld and Pandis* (1998)
S 18	$HSO_3^- + HSO_5^- \xrightarrow{H^+} SO_4^{2-} + SO_4^{2-} + H^+ + H^+$	7.1 x 10^6		*Betterton and Hoffmann* (1988)
S 19	$SO_4^- + OH \longrightarrow HSO_5^-$	1.0 x 10^9		*Jiang et al.* (1992)
S 20	$SO_4^- + HO_2 \longrightarrow SO_4^{2-} + H^+$	3.5 x 10^9		*Jiang et al.* (1992)
S 21	$SO_4^- + O_2^- \longrightarrow SO_4^{2-}$	3.5 x 10^9		assumed =S20
S 22	$SO_4^- + H_2O \longrightarrow SO_4^{2-} + H^+ + OH$	1.1 x 10^1	-1110	*Herrmann et al.* (1995)
S 23	$SO_4^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+ + HO_2$	1.2 x 10^7		*Wine et al.* (1989)
S 24	$SO_4^- + NO_3^- \longrightarrow SO_4^{2-} + NO_3$	5.0 x 10^4		*Exner et al.* (1992)
S 25	$SO_4^- + HSO_3^- \longrightarrow SO_3^- + SO_4^{2-} + H^+$	8.0 x 10^8		*Huie and Neta* (1987)
S 26	$SO_4^- + SO_3^{2-} \longrightarrow SO_3^- + SO_4^{2-}$	4.6 x 10^8		*Huie and Neta* (1987)
S 27	$SO_4^{2-} + NO_3 \longrightarrow NO_3^- + SO_4^-$	1.0 x 10^5		*Logager et al.* (1993)
S 28	$SO_5^- + HSO_3^- \longrightarrow SO_4^- + SO_4^{2-} + H^+$	7.5 x 10^4		*Huie and Neta* (1987)
S 29	$SO_5^- + SO_3^{2-} \longrightarrow SO_4^- + SO_4^{2-}$	9.4 x 10^6		*Huie and Neta* (1987)
S 30	$SO_5^- + HSO_3^- \longrightarrow SO_3^- + HSO_5^-$	2.5 x 10^4		*Huie and Neta* (1987); *Deister and Warneck* (1990)
S 31	$SO_5^- + SO_3^{2-} \xrightarrow{H^+} SO_3^- + HSO_5^-$	3.6 x 10^6		*Huie and Neta* (1987); *Deister and Warneck* (1990)
S 32	$SO_5^- + O_2^- \xrightarrow{H^+} HSO_5^- + O_2$	2.3 x 10^8		*Buxton et al.* (1996)
S 33	$SO_5^- + SO_5^- \longrightarrow H_2O$	1.0 x 10^8		*Ross et al.* (1992)

Table 3: Continued.

no	reaction	k_0 [(M^{1-n})s^{-1}]	$-E_a$ / R [K]	reference
S 34	$DMS + O_3 \longrightarrow O_2 + DMSO$	8.6 x 10^{8}	-2600	*Gershenzon et al.* (2001)
S 35	$DMS + OH \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH3OO + 0.5\ HSO_4^- + HCHO + H^+$	1.9 x 10^{10}		*Ross et al.* (1998)
S 36	$DMSO + OH \longrightarrow CH_3SO_2^- + CH3OO + H^+$	4.5 x 10^{9}		*Bardouki et al.* (2002)
S 37	$CH_3SO_2^- + OH \longrightarrow CH_3SO_3^-$ +H2O - O2	1.2 x 10^{10}		*Bardouki et al.* (2002)
S 38	$CH_3SO_3^- + OH \longrightarrow SO_4^{2-} + H^+ + CH3OO$	1.2 x 10^{7}		*Bonsang et al.* (1991)
Cl 1	$Cl + H_2O_2 \longrightarrow HO_2 + Cl^- + H^+$	2.0 x 10^{9}		*Yu* (2001)
Cl 2	$Cl + H_2O \longrightarrow H^+ + ClOH^-$	1.8 x 10^{5}		*Yu* (2001)
Cl 3	$Cl + NO_3^- \longrightarrow NO_3 + Cl^-$	1.0 x 10^{8}		*Buxton et al.* (1999b)
Cl 4	$Cl + DOM \longrightarrow Cl^- + HO_2$	5.0 x 10^{9}		estimated by *Anastasio et al.* (2003) from *Ross et al.* (1998)
Cl 5	$Cl + SO_4^{2-} \longrightarrow SO_4^- + Cl^-$	2.1 x 10^{8}		*Buxton et al.* (1999a)
Cl 6	$Cl + Cl \longrightarrow Cl_2$	8.8 x 10^{7}		*Wu et al.* (1980)
Cl 7	$Cl^- + OH \longrightarrow ClOH^-$	4.2 x 10^{9}		*Yu* (2001)
Cl 8	$Cl^- + O_3 \longrightarrow ClO^- + O_2$	3.0 x 10^{-3}		*Hoigné et al.* (1985)
Cl 9	$Cl^- + NO_3 \longrightarrow NO_3^- + Cl$	9.3 x 10^{6}	-4330	*Exner et al.* (1992)
Cl 10	$Cl^- + SO_4^- \longrightarrow SO_4^{2-} + Cl$	2.5 x 10^{8}		*Buxton et al.* (1999a)
Cl 11	$Cl^- + HSO_5^- \longrightarrow HOCl + SO_4^{2-}$	1.8 x 10^{-3}	-7352	*Fortnum et al.* (1960)
Cl 12	$Cl^- + HOCl + H^+ \longrightarrow Cl_2$	2.2 x 10^{4}	-3508	*Ayers et al.* (1996)
Cl 13	$Cl_2 \longrightarrow Cl^- + HOCl + H^+$	2.2 x 10^{1}	-8012	*Ayers et al.* (1996)
Cl 14	$Cl_2^- + OH \longrightarrow HOCl + Cl^-$	1.0 x 10^{9}		*Ross et al.* (1998)
Cl 15	$Cl_2^- + OH^- \longrightarrow Cl^- + Cl^- + OH$	4.0 x 10^{6}		*Jacobi* (1996)
Cl 16	$Cl_2^- + HO_2 \longrightarrow Cl^- + Cl^- + H^+ + O_2$	3.1 x 10^{9}		*Yu* (2001)
Cl 17	$Cl_2^- + O_2^- \longrightarrow Cl^- + Cl^- + O_2$	6.0 x 10^{9}		*Jacobi* (1996)
Cl 18	$Cl_2^- + H_2O_2 \longrightarrow Cl^- + Cl^- + H^+ + HO_2$	7.0 x 10^{5}	-3340	*Jacobi* (1996)
Cl 19	$Cl_2^- + NO_2^- \longrightarrow Cl^- + Cl^- + NO_2$	6.0 x 10^{7}		*Jacobi* (1996)
Cl 20	$Cl_2^- + CH_3OOH \longrightarrow Cl^- + Cl^- + H^+ + CH3OO$	7.0 x 10^{5}	-3340	assumed by *Jacobi* (1996)
Cl 21	$Cl_2^- + DOM \longrightarrow Cl^- + Cl^- + HO_2$	1.0 x 10^{6}		estimated by *Anastasio et al.* (2003) from *Ross et al.* (1998)
Cl 22	$Cl_2^- + HSO_3^- \longrightarrow SO_3^- + Cl^- + Cl^- + H^+$	4.7 x 10^{8}	-1082	*Shoute et al.* (1991)
Cl 23	$Cl_2^- + SO_3^{2-} \longrightarrow SO_3^- + Cl^- + Cl^-$	6.2 x 10^{7}		*Jacobi et al.* (1996)
Cl 24	$Cl_2^- + Cl_2^- \longrightarrow Cl_2 + 2Cl^-$	6.2 x 10^{9}		*Yu* (2001)
Cl 25	$Cl_2^- + Cl \longrightarrow Cl^- + Cl_2$	2.7 x 10^{9}		*Yu* (2001)
Cl 26	$Cl_2^- + DMS \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH3OO + 0.5\ HSO_4^- + HCHO + 2\ Cl^- + 2\ H^+$	3.0 x 10^{9}		rate from *Ross et al.* (1998)
Cl 27	$ClOH^- \longrightarrow Cl^- + OH$	6.0 x 10^{9}		*Yu* (2001)
Cl 28	$ClOH^- + H^+ \longrightarrow Cl$	4.0 x 10^{10}		*Yu* (2001)

Table 3: Continued.

no	reaction	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
Cl 29	$HOCl + HO_2 \longrightarrow Cl + O_2$	7.5 x 10^6		assumed = Cl30 *Long and Bielski* (1980)
Cl 30	$HOCl + O_2^- \longrightarrow Cl + OH^- + O_2$	7.5 x 10^6		*Long and Bielski* (1980)
Cl 31	$HOCl + SO_3^{2-} \longrightarrow Cl^- + HSO_4^-$	7.6 x 10^8		*Fogelman et al.* (1989)
Cl 32	$HOCl + HSO_3^- \longrightarrow Cl^- + HSO_4^- + H^+$	7.6 x 10^8		assumed = Cl31 *Fogelman et al.* (1989)
Cl 33	$Cl_2 + HO_2 \longrightarrow Cl_2^- + H^+ + O_2$	1.0 x 10^9		*Bjergbakke et al.* (1981)
Cl 34	$Cl_2 + O_2^- \longrightarrow Cl_2^- + O_2$	1.0 x 10^9		assumed = Cl33 *Bjergbakke et al.* (1981)
Br 1	$Br + OH^- \longrightarrow BrOH^-$	1.3 x 10^{10}		*Zehavi and Rabani* (1972)
Br 2	$Br + DOM \longrightarrow Br^- + HO_2$	2.0 x 10^8		estimated by *Anastasio et al.* (2003) from *Ross et al.* (1998)
Br 3	$Br^- + OH \longrightarrow BrOH^-$	1.1 x 10^{10}		*Zehavi and Rabani* (1972)
Br 4	$Br^- + O_3 \longrightarrow BrO^-$	2.1 x 10^2	-4450	*Haag and Hoigné* (1983)
Br 5	$Br^- + NO_3 \longrightarrow Br + NO_3^-$	3.8 x 10^9		Zellner et al. 1996 in *Herrmann et al.* (2000)
Br 6	$Br^- + SO_4^- \longrightarrow Br + SO_4^{2-}$	2.1 x 10^9		*Jacobi* (1996)
Br 7	$Br^- + HSO_5^- \longrightarrow HOBr + SO_4^{2-}$	1.0	-5338	*Fortnum et al.* (1960)
Br 8	$Br^- + HOBr + H^+ \longrightarrow Br_2$	1.6 x 10^{10}		*Liu and Margerum* (2001)
Br 9	$Br_2 \longrightarrow Br^- + HOBr + H^+$	9.7 x 10^1	7457	*Liu and Margerum* (2001)
Br 10	$Br_2^- + O_2^- \longrightarrow Br^- + Br^-$	1.7 x 10^8		*Wagner and Strehlow* (1987)
Br 11	$Br_2^- + HO_2 \longrightarrow Br_2 + H_2O_2$ - H^+	4.4 x 10^9		*Matthew et al.* (2003)
Br 12	$Br_2^- + H_2O_2 \longrightarrow Br^- + Br^- + H^+ + HO_2$	5.0 x 10^2		*Chameides and Stelson* (1992)
Br 13	$Br_2^- + Br_2^- \longrightarrow Br^- + Br^- + Br_2$	1.9 x 10^9		*Ross et al.* (1992)
Br 14	$Br_2^- + CH_3OOH \longrightarrow Br^- + Br^- + H^+ + CH3OO$	1.0 x 10^5		assumed by *Jacobi* (1996)
Br 15	$Br_2^- + DOM \longrightarrow Br^- + Br^- + HO_2$	1.0 x 10^5		estimated by *Anastasio et al.* (2003) from *Ross et al.* (1998)
Br 16	$Br_2^- + NO_2^- \longrightarrow Br^- + Br^- + NO_2$	1.7 x 10^7	-1720	*Shoute et al.* (1991)
Br 17	$Br_2^- + HSO_3^- \longrightarrow Br^- + Br^- + H^+ + SO_3^-$	6.3 x 10^7	-782	*Shoute et al.* (1991)
Br 18	$Br_2^- + SO_3^{2-} \longrightarrow Br^- + Br^- + SO_3^-$	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 $HSO_4^- + HCHO + 2\ Br^- + 2\ H^+$	3.2 x 10^9		rate from *Ross et al.* (1998)
Br 20	$BrOH^- \longrightarrow Br^- + OH$	3.3 x 10^7		*Zehavi and Rabani* (1972)
Br 21	$BrOH^- \longrightarrow Br + OH^-$	4.2 x 10^6		*Zehavi and Rabani* (1972)
Br 22	$BrOH^- + H^+ \longrightarrow Br$	4.4 x 10^{10}		*Zehavi and Rabani* (1972)
Br 23	$BrOH^- + Br^- \longrightarrow Br_2^- + OH^-$	1.9 x 10^8		*Zehavi and Rabani* (1972)
Br 24	$BrO^- + SO_3^{2-} \longrightarrow Br^- + SO_4^{2-}$	1.0 x 10^8		*Troy and Margerum* (1991)
Br 25	$HOBr + HO_2 \longrightarrow Br + O_2$	1.0 x 10^9		*Herrmann et al.* (1999)
Br 26	$HOBr + O_2^- \longrightarrow Br + OH^- + O_2$	3.5 x 10^9		*Schwarz and Bielski* (1986)

Table 3: Continued.

no	reaction	k_0 [$(M^{1-n})s^{-1}$]	$-E_a$ / R [K]	reference
Br 27	$HOBr + H_2O_2 \longrightarrow Br^- + H^+ + O_2$	1.2 x 10^6		*von Gunten and Oliveras* (1998)
Br 28	$HOBr + SO_3^{2-} \longrightarrow Br^- + HSO_4^-$	5.0 x 10^9		*Troy and Margerum* (1991)
Br 29	$HOBr + HSO_3^- \longrightarrow Br^- + HSO_4^- + H^+$	5.0 x 10^9		assumed = Br28
Br 30	$Br_2 + HO_2 \longrightarrow Br_2^- + H^+ + O_2$	1.1 x 10^8		*Ross et al.* (1998)
Br 31	$Br_2 + O_2^- \longrightarrow Br_2^- + O_2$	5.6 x 10^9		*Ross et al.* (1998)
Hx 1	$Br^- + HOCl + H^+ \longrightarrow BrCl$	1.3 x 10^6		*Liu and Margerum* (2001)
Hx 2	$Cl^- + HOBr + H^+ \longrightarrow BrCl$	2.3 x 10^{10}		*Liu and Margerum* (2001)
Hx 3	$BrCl \longrightarrow Cl^- + HOBr + H^+$	3.0 x 10^6		*Liu and Margerum* (2001)
Hx 4	$Br^- + ClO^- + H^+ \longrightarrow BrCl + OH^-$	3.7 x 10^{10}		*Kumar and Margerum* (1987)
Hx 5	$Cl_2 + Br^- \longrightarrow BrCl_2^-$	7.7 x 10^9		*Liu and Margerum* (2001)
Hx 6	$BrCl_2^- \longrightarrow Cl_2 + Br^-$	1.83 x 10^3		*Liu and Margerum* (2001)
hv 1	$O_3 + hv \longrightarrow OH + OH + O_2$			assumed 2x gas phase
hv 2	$H_2O_2 + hv \longrightarrow OH + OH$			assumed 2x gas phase
hv 3	$NO_3^- + hv \xrightarrow{H^+} NO_2 + OH$			*Zellner et al.* (1990)
hv 4	$NO_2^- + hv \xrightarrow{H^+} NO + OH$			*Zellner et al.* (1990); *Burley and Johnston* (1992)
hv 5	$HOCl + hv \longrightarrow OH + Cl$			assumed 2x gas phase
hv 6	$Cl_2 + hv \longrightarrow Cl + Cl$			assumed 2x gas phase
hv 7	$HOBr + hv \longrightarrow OH + Br$			assumed 2x gas phase
hv 8	$Br_2 + hv \longrightarrow Br + Br$			assumed 2x gas phase
hv 9	$BrCl + hv \longrightarrow Cl + Br$			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
H1	$N_2O_5 \xrightarrow{H_2O} HNO_{3aq} + HNO_{3aq}$	$\overline{k_t}(N_2O_5)w_{l,i}[H_2O]/Het_T$	*Behnke et al.* (1994), *Behnke et al.* (1997)
H2	$N_2O_5 \xrightarrow{Cl^-} ClNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	*Behnke et al.* (1994), *Behnke et al.* (1997)
H3	$N_2O_5 \xrightarrow{Br^-} BrNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Br^-)[Br^-]/Het_T$	*Behnke et al.* (1994), *Behnke et al.* (1997)
H4	$ClNO_3 \xrightarrow{H_2O} HOCl_{aq} + HNO_{3aq}$	$\overline{k_t}(ClNO_3)w_{l,i}[H_2O]/Het_T$	see note
H5	$ClNO_3 \xrightarrow{Cl^-} Cl_{2aq} + NO_3^-$	$\overline{k_t}(ClNO_3)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	see note
H6	$ClNO_3 \xrightarrow{Br^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(ClNO_3)w_{l,i}f(Br^-)[Br^-]/Het_T$	see note
H7	$BrNO_3 \xrightarrow{H_2O} HOBr_{aq} + HNO_{3aq}$	$\overline{k_t}(BrNO_3)w_{l,i}[H_2O]/Het_T$	see note
H8	$BrNO_3 \xrightarrow{Cl^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(BrNO_3)w_{l,i}f(Cl^-)[Cl^-]/Het_T$	see note
H9	$BrNO_3 \xrightarrow{Br^-} Br_{2aq} + NO_3^-$	$\overline{k_t}(BrNO_3)w_{l,i}f(Br^-)[Br^-]/Het_T$	see note

For a definition of $\overline{k_t}$ and $w_{l,i}$ see *von Glasow et al.* (2002) 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
EQ1	$CO_{2aq} \longleftrightarrow H^+ + HCO_3^-$	1	2	4.3×10^{-7}	-913	*Chameides* (1984)
EQ2	$NH_{3aq} \longleftrightarrow OH^- + NH_4^+$	1	2	1.7×10^{-5}	-4325	*Chameides* (1984)
EQ3	$H_2O_{aq} \longleftrightarrow H^+ + OH^-$	1	2	1.0×10^{-14}	-6716	*Chameides* (1984)
EQ4	$HCOOH_{aq} \longleftrightarrow H^+ + HCOO^-$	1	2	1.8×10^{-4}		*Weast* (1980)
EQ5	$HSO_3^- \longleftrightarrow H^+ + SO_3^{2-}$	1	2	6.0×10^{-8}	1120	*Chameides* (1984)
EQ6	$H_2SO_{4aq} \longleftrightarrow H^+ + HSO_4^-$	1	2	1.0×10^{3}		*Seinfeld and Pandis* (1998)
EQ7	$HSO_4^- \longleftrightarrow H^+ + SO_4^{2-}$	1	2	1.2×10^{-2}	1120	*Weast* (1980)
EQ8	$HO_{2aq} \longleftrightarrow O_2^- + H^+$	1	2	1.6×10^{-5}		*Weinstein-Lloyd and Schwartz* (1991)
EQ9	$SO_{2aq} \longleftrightarrow H^+ + HSO_3^-$	1	2	1.7×10^{-2}	2090	*Chameides* (1984)
EQ10	$Cl_2^- \longleftrightarrow Cl_{aq} + Cl^-$	1	2	5.2×10^{-6}		*Jayson et al.* (1973)
EQ11	$HOCl_{aq} \longleftrightarrow H^+ + ClO^-$	1	2	3.2×10^{-8}		*Lax* (1969)
EQ12	$HBr_{aq} \longleftrightarrow H^+ + Br^-$	1	2	1.0×10^{9}		*Lax* (1969)
EQ13	$Br_2^- \longleftrightarrow Br_{aq} + Br^-$	1	2	9.1×10^{-6}		*Mamou et al.* (1977)
EQ14	$HOBr_{aq} \longleftrightarrow H^+ + BrO^-$	1	2	2.3×10^{-9}	-3091	*Kelley and Tartar* (1956)
EQ15	$BrCl_{aq} + Cl^- \longleftrightarrow BrCl_2^-$	2	1	3.8	1143	*Wang et al.* (1994)
EQ16	$BrCl_{aq} + Br^- \longleftrightarrow Br_2Cl^-$	2	1	1.8×10^{4}		*Wang et al.* (1994)
EQ17	$Br_{2aq} + Cl^- \longleftrightarrow Br_2Cl^-$	2	1	1.3		*Wang et al.* (1994)
EQ18	$HNO_{3aq} \longleftrightarrow H^+ + NO_3^-$	1	2	1.5×10^{1}		*Davis and de Bruin* (1964)
EQ19	$HCl_{aq} \longleftrightarrow H^+ + Cl^-$	1	2	1.7×10^{6}		*Marsh and McElroy* (1985)
EQ20	$HONO_{aq} \longleftrightarrow H^+ + NO_2^-$	1	2	5.1×10^{-4}	-1260	*Schwartz and White* (1981)
EQ21	$HNO_{4aq} \longleftrightarrow NO_4^- + H^+$	1	2	1.0×10^{-5}	8700	*Warneck* (1999)

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)

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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