

Technical notes: Kinetic data for MISTRA

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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 in MISTRA

Gas phase
O ¹ D, O ₂ , O ₃ , OH, HO ₂ , H ₂ O ₂ , H ₂ O
NO, NO ₂ , NO ₃ , N ₂ O ₅ , HONO, HNO ₃ , HNO ₄ , PAN, NH ₃ , RONO ₂
CO, CO ₂ , CH ₄ , C ₂ H ₆ , C ₂ H ₄ , HCHO, HCOOH, ALD (i.e., CH ₃ CHO), CH ₂ O ₂ , HOCH ₂ O ₂ , CH ₃ CO ₃ , CH ₃ O ₂ , C ₂ H ₅ O ₂ , H ₃ CO ₂ , EO ₂ (i.e., H ₂ C(OH)CH ₂ OO), CH ₂ O ₂ , ROOH (i.e., alkylhydroperoxides), DOM
SO ₂ , SO ₃ , HOSO ₂ , H ₂ SO ₄ , DMS, CH ₃ SCH ₂ OO, DMSO, DMSO ₂ , CH ₃ S, CH ₃ SO, CH ₃ SO ₂ , CH ₃ SO ₃ , CH ₃ SO ₂ H, CH ₃ SO ₃ H
Cl, ClO, OClO, HCl, HOCl, Cl ₂ , Cl ₂ O ₂ , ClNO ₂ , ClNO ₃
Br, BrO, HBr, HOBr, Br ₂ , BrNO ₂ , BrNO ₃ , BrCl, CHBr ₃ , CH ₃ Br
Liquid phase (neutral)
O ₂ , O ₃ , OH, HO ₂ , H ₂ O ₂ , H ₂ O
NO, NO ₂ , NO ₃ , HONO, HNO ₃ , HNO ₄ , NH ₃
CO ₂ , HCHO, HCOOH, CH ₃ OH, CH ₃ OO, CH ₃ OOH
SO ₂ , H ₂ SO ₄ , DMSO, DMSO ₂ , CH ₃ SO ₂ H, CH ₃ SO ₃ H
Cl, HCl, HOCl, Cl ₂
Br, HBr, HOBr, Br ₂ , BrCl
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 ₃ SO ₃ ⁻ , CH ₂ OHSO ₂ ⁻ , CH ₂ OHSO ₃ ⁻
Cl ⁻ , Cl ₂ ⁻ , ClO ⁻ , ClOH ⁻
Br ⁻ , Br ₂ ⁻ , BrO ⁻ , BrCl ₂ ⁻ , Br ₂ Cl ⁻ , BrOH ⁻

Table 2: Gas phase reactions.

no	reaction	n	$A [(\text{cm}^{-3})^{1-n} \text{s}^{-1}]$	$-E_a / R$ [K]	reference
O 1	$\text{O}^1\text{D} + \text{O}_2 \longrightarrow \text{O}_3$	2	3.2×10^{-11}	70	Atkinson et al. (2006)
O 2	$\text{O}^1\text{D} + \text{N}_2 \longrightarrow \text{O}_3$	2	1.8×10^{-11}	110	Atkinson et al. (2006)
O 3	$\text{O}^1\text{D} + \text{H}_2\text{O} \longrightarrow 2 \text{OH}$	2	2.2×10^{-10}		Atkinson et al. (2006)
O 4	$\text{OH} + \text{O}_3 \longrightarrow \text{HO}_2 + \text{O}_2$	2	1.7×10^{-12}	-940	Atkinson et al. (2006)
O 5	$\text{OH} + \text{HO}_2 \longrightarrow \text{H}_2\text{O} + \text{O}_2$	2	4.8×10^{-11}	250	Atkinson et al. (2006)
O 6	$\text{OH} + \text{H}_2\text{O}_2 \longrightarrow \text{HO}_2 + \text{H}_2\text{O}$	2	2.9×10^{-12}	-160	Atkinson et al. (2006)
O 7	$\text{HO}_2 + \text{O}_3 \longrightarrow \text{OH} + 2\text{O}_2$	2	1.0×10^{-14}	-490	Atkinson et al. (2004)
O 8	$\text{HO}_2 + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{O}_2$	2	2.3×10^{-13}	600	Atkinson et al. (2006)
O 9	$\text{O}_3 + h\nu \longrightarrow \text{O}_2 + \text{O}^1\text{D}$	1	1		DeMore et al. (1997)
O 10	$\text{H}_2\text{O}_2 + h\nu \longrightarrow 2\text{OH}$	1	1		DeMore et al. (1997)
N 1	$\text{NO} + \text{OH} \xrightarrow{M} \text{HONO}$	3	2		Sander et al. (2003)
N 2	$\text{NO} + \text{HO}_2 \longrightarrow \text{NO}_2 + \text{OH}$	2	3.5×10^{-12}	250	Atkinson et al. (2004)
N 3	$\text{NO} + \text{O}_3 \longrightarrow \text{NO}_2 + \text{O}_2$	2	3.0×10^{-12}	-1500	Sander et al. (2003)
N 4	$\text{NO} + \text{NO}_3 \longrightarrow 2\text{NO}_2$	2	1.5×10^{-11}	170	Sander et al. (2003)
N 5	$\text{NO}_2 + \text{OH} \xrightarrow{M} \text{HNO}_3$	3	2		Sander et al. (2003)
N 6	$\text{NO}_2 + \text{HO}_2 \xrightarrow{M} \text{HNO}_4$	3	2		Atkinson et al. (2006)
N 7	$\text{NO}_2 + \text{O}_3 \longrightarrow \text{NO}_3 + \text{O}_2$	2	1.2×10^{-13}	-2450	Sander et al. (2003)
N 8	$\text{NO}_2 + h\nu \longrightarrow \text{NO} + \text{O}_3$	1	1		DeMore et al. (1997)
N 9	$\text{NO}_2 + \text{NO}_3 \xrightarrow{M} \text{N}_2\text{O}_5$	3	2		Sander et al. (2003)
N 10	$\text{NO}_3 + h\nu \longrightarrow \text{NO} + \text{O}_2$	1	1		Wayne et al. (1991)
N 11	$\text{NO}_3 + \text{HO}_2 \longrightarrow 0.3 \text{HNO}_3 + 0.7 \text{OH} + 0.7 \text{NO}_2 + \text{O}_2$	2	4.0×10^{-12}		Atkinson et al. (2006)
N 12	$\text{NO}_3 + \text{NO}_3 \longrightarrow \text{NO}_2 + \text{NO}_2 + \text{O}_2$	2	8.5×10^{-13}	-2450	Sander et al. (2003)
N 13	$\text{NO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{O}_3$	1	1		Wayne et al. (1991)
N 14	$\text{N}_2\text{O}_5 \xrightarrow{M} \text{NO}_2 + \text{NO}_3$	2	2		Sander et al. (2003)
N 15	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \longrightarrow 2\text{HNO}_3$	2	2.6×10^{-22}		Atkinson et al. (2006)
N 16	$\text{N}_2\text{O}_5 + h\nu \longrightarrow \text{NO}_2 + \text{NO}_3$	1	1		DeMore et al. (1997)
N 17	$\text{HONO} + \text{OH} \longrightarrow \text{NO}_2$	2	1.8×10^{-11}	-390	Sander et al. (2003)
N 18	$\text{HONO} + h\nu \longrightarrow \text{NO} + \text{OH}$	1	1		DeMore et al. (1997)
N 19	$\text{HNO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{OH}$	1	1		DeMore et al. (1997)
N 20	$\text{HNO}_3 + \text{OH} \longrightarrow \text{NO}_3 + \text{H}_2\text{O}$	2	2		Atkinson et al. (2006)
N 21	$\text{HNO}_4 \xrightarrow{M} \text{NO}_2 + \text{HO}_2$	2	2		Sander et al. (2003)
N 22	$\text{HNO}_4 + \text{OH} \longrightarrow \text{NO}_2 + \text{H}_2\text{O} + \text{O}_2$	2	1.3×10^{-12}	380	Haggerstone et al. (2005)
N 23	$\text{HNO}_4 + h\nu \longrightarrow \text{NO}_2 + \text{HO}_2$	1	1		DeMore et al. (1997)
N 24	$\text{HNO}_4 + h\nu \longrightarrow \text{OH} + \text{NO}_3$	1	1		DeMore et al. (1997)
N 25	$\text{RONO}_2 + \text{OH} \longrightarrow \text{R} + \text{H}_2\text{O} + \text{NO}_2$	2	1.3×10^{-12}		Sander et al. (1997)
N 26	$\text{RONO}_2 + h\nu \longrightarrow \text{RO} + \text{NO}_2$	1	assumed similar as N 19		Sander et al. (1997)

Table 2: Continued.

no	reaction	n	A [(cm ⁻³) ¹⁻ⁿ 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 ₃ OO + H ₂ O	2	2.4×10^{-12}	-1775	Sander et al. (2003)
C 3	C ₂ H ₆ + OH \rightarrow C ₂ H ₅ O ₂ + H ₂ O	2	1.7×10^{-11}	-1232	Lurmann et al. (1986)
C 4	C ₂ H ₄ + OH \rightarrow EO ₂	2	1.66×10^{-12}	474	Sander et al. (1997), see note
C 5	C ₂ H ₄ + O ₃ \rightarrow HCHO + 0.4CH ₂ O 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 ₃ OO \rightarrow ROOH + O ₂	2	4.1×10^{-13}	750	Sander et al. (2003)
C 7	HO ₂ + C ₂ H ₅ O ₂ \rightarrow ROOH + O ₂	2	7.5×10^{-13}	700	Sander et al. (2003)
C 8	HO ₂ + CH ₃ CO ₃ \rightarrow ROOH + O ₂	2	4.5×10^{-13}	1000	DeMore et al. (1997)
C 9	CH ₃ OO + CH ₃ OO \rightarrow 1.4HCHO + 0.8HO ₂ + O ₂	2	1.5×10^{-13}	220	Lurmann et al. (1986)
C 10	C ₂ H ₅ O ₂ + NO \rightarrow ALD + HO ₂ + NO ₂	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 11	2C ₂ H ₅ O ₂ \rightarrow 1.6ALD + 1.2HO ₂	2	5.00×10^{-14}		Lurmann et al. (1986)
C 12	EO ₂ + NO \rightarrow NO ₂ + 2.0HCHO + HO ₂	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 13	EO ₂ + EO ₂ \rightarrow 2.4HCHO + 1.2HO ₂ + 0.4ALD	2	5.00×10^{-14}		Lurmann et al. (1986)
C 14	HO ₂ + EO ₂ \rightarrow ROOH + O ₂	2	3.00×10^{-12}		Lurmann et al. (1986)
C 15	HCHO + hν \rightarrow 2HO ₂ + CO	1	1		DeMore et al. (1997)
C 16	HCHO + hν \rightarrow CO + H ₂	1	1		DeMore et al. (1997)
C 17	HCHO + OH $\xrightarrow{O_2}$ HO ₂ + CO + H ₂ O	2	1.00×10^{-11}		DeMore et al. (1997)
C 18	HCHO + HO ₂ \rightarrow HOCH ₂ O 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 \rightarrow CH ₃ CO ₃ + H ₂ O	2	6.9×10^{-12}	250	Lurmann et al. (1986)
C 21	ALD + NO ₃ \rightarrow HNO ₃ + CH ₃ CO ₃	2	1.40×10^{-15}		DeMore et al. (1997)
C 22	ALD + hν \rightarrow CH ₃ OO + HO ₂ + CO	1	1		Lurmann et al. (1986)
C 23	ALD + hν \rightarrow CH ₄ + CO	1	1		Lurmann et al. (1986)
C 24	HOCH ₂ O ₂ + NO \rightarrow HCOOH + HO ₂ + NO ₂	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 25	HOCH ₂ O ₂ + HO ₂ \rightarrow HCOOH + H ₂ O + O ₂	2	2.00×10^{-12}		Lurmann et al. (1986)
C 26	2 HOCH ₂ O ₂ \rightarrow 2HCOOH + 2HO ₂ + 2O ₂	2	1.00×10^{-13}		Lurmann et al. (1986)
C 27	HCOOH + OH $\xrightarrow{O_2}$ HO ₂ + H ₂ O + CO ₂	2	4.0×10^{-13}		DeMore et al. (1997)
C 28	CH ₃ CO ₃ + NO ₂ \rightarrow PAN	2	4.70×10^{-12}		Lurmann et al. (1986)
C 29	PAN \rightarrow CH ₃ CO ₃ + NO ₂	1	1.9×10^{16}	-13543	DeMore et al. (1997)
C 30	CH ₃ CO ₃ + NO $\xrightarrow{O_2}$ CH ₃ OO + NO ₂ + CO ₂	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C 31	CH ₃ OO + NO $\xrightarrow{O_2}$ HCHO + NO ₂ + HO ₂	2	3.0×10^{-12}	280	DeMore et al. (1997)
C 32	ROOH + OH \rightarrow 0.7 CH ₃ OO + 0.3 HCHO + 0.3 OH	2	3.8×10^{-12}	200	DeMore et al. (1997), see note
C 33	ROOH + hν \rightarrow 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	$\text{SO}_2 + \text{OH} \xrightarrow{M} \text{HOSO}_2$	3	2		Atkinson et al. (2006)
S 2	$\text{HOSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_3$	2	1.3×10^{-12}	330	Atkinson et al. (2006)
S 3	$\text{SO}_3 \xrightarrow{\text{H}_2\text{O}} \text{H}_2\text{SO}_4$	1	2		Jayne et al. (1997)
S 4	$\text{CH}_3\text{SCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{SCH}_2\text{OO} + \text{H}_2\text{O}$	2	2		Atkinson et al. (1997)
S 5	$\text{CH}_3\text{SCH}_3 + \text{OH} \xrightarrow{\text{O}_2} \text{CH}_3\text{SOCH}_3 + \text{HO}_2$	2	2		Atkinson et al. (1997)
S 6	$\text{CH}_3\text{SCH}_3 + \text{NO}_3 \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HNO}_3$	2	1.9×10^{-13}	520	Atkinson et al. (1999)
S 7	$\text{CH}_3\text{SCH}_3 + \text{Cl} \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HCl}$	2	3.3×10^{-10}		Atkinson et al. (1999)
S 8	$\text{CH}_3\text{SCH}_3 + \text{Br} \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HBr}$	2	9.0×10^{-11}	-2386	Jefferson et al. (1994)
S 9	$\text{CH}_3\text{SCH}_3 + \text{BrO} \rightarrow \text{CH}_3\text{SOCH}_3 + \text{Br}$	2	2.54×10^{-14}	850	Ingham et al. (1999)
S 10	$\text{CH}_3\text{SCH}_3 + \text{ClO} \rightarrow \text{CH}_3\text{SOCH}_3 + \text{Cl}$	2	9.5×10^{-15}		Barnes et al. (1991)
S 11	$\text{CH}_3\text{SCH}_3 + \text{IO} \rightarrow \text{CH}_3\text{SOCH}_3 + \text{I}$	2	1.4×10^{-14}		THALOZ (2005)
S 12	$\text{CH}_3\text{SCH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{CH}_3\text{S} + \text{NO}_2$	2	4.9×10^{-12}	263	Urbanski et al. (1997)
S 13	$\text{CH}_3\text{SCH}_2\text{OO} + \text{CH}_3\text{SCH}_2\text{OO} \xrightarrow{\text{O}_2} 2 \text{HCHO} + 2 \text{CH}_3\text{S}$	2	1.0×10^{-11}		Urbanski et al. (1997); Atkinson et al. (2006)
S 14	$\text{CH}_3\text{S} + \text{O}_3 \rightarrow \text{CH}_3\text{SO} + \text{O}_2$	2	1.15×10^{-12}	432	Atkinson et al. (2006)
S 15	$\text{CH}_3\text{S} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO} + \text{NO}$	2	3.0×10^{-11}	210	Atkinson et al. (2006)
S 16	$\text{CH}_3\text{SO} + \text{NO}_2 \xrightarrow{\text{O}_2} 0.82 \text{CH}_3\text{SO}_2 + 0.18 \text{SO}_2 + 0.18 \text{H}_3\text{CO}_2 + \text{NO}$	2	1.2×10^{-11}		Atkinson et al. (2006); Kukui et al. (2000), product ratios from van Dingenen et al. (1994)
S 17	$\text{CH}_3\text{SO} + \text{O}_3 \xrightarrow{\text{O}_2} \text{CH}_3\text{SO}_2$	2	6.0×10^{-13}		Atkinson et al. (2006)
S 18	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{OO}$	1	1.9×10^{13}	-8661	Barone et al. (1995)
S 19	$\text{CH}_3\text{SO}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{NO}$	2	2.2×10^{-12}		Ray et al. (1996)
S 20	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	2	$3. \times 10^{-13}$		Barone et al. (1995)
S 21	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	2	$5. \times 10^{-11}$		Barone et al. (1995)
S 22	$\text{CH}_3\text{SO}_3 \xrightarrow{\text{H}_2\text{O}, \text{O}_2} \text{CH}_3\text{OO} + \text{H}_2\text{SO}_4$	1	1.36×10^{14}	-11071	Barone et al. (1995)
S 23	$\text{CH}_3\text{SOCH}_3 + \text{OH} \rightarrow 0.95 \text{CH}_3\text{SO}_2\text{H} + 0.95 \text{CH}_3\text{OO} + 0.05 \text{DMSO}_2$	2	8.7×10^{-11}		Urbanski et al. (1998)
S 24	$\text{CH}_3\text{SO}_2\text{H} + \text{OH} \rightarrow 0.95 \text{CH}_3\text{SO}_2 + 0.05 \text{CH}_3\text{SO}_3\text{H} + 0.05 \text{HO}_2 + \text{H}_2\text{O}$	2	$9. \times 10^{-11}$		Kukui et al. (2003)
S 25	$\text{CH}_3\text{SO}_2\text{H} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3$	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 → ClO + O ₂	2	2.8 × 10 ⁻¹¹	-250	Atkinson et al. (2006)
Cl 2	Cl + HO ₂ → HCl + O ₂	2	1.8 × 10 ⁻¹¹	170	Sander et al. (2003)
Cl 3	Cl + HO ₂ → ClO + OH	2	4.1 × 10 ⁻¹¹	-450	Sander et al. (2003)
Cl 4	Cl + H ₂ O ₂ → HCl + HO ₂	2	1.1 × 10 ⁻¹¹	-980	Atkinson et al. (2006)
Cl 5	Cl + CH ₃ OO → 0.5 ClO + 0.5 HCHO + 0.5 HO ₂ + 0.5 HCl + 0.5 CO + 0.5 H ₂ O	2	1.6 × 10 ⁻¹⁰		Sander et al. (2003)
Cl 6	Cl + NO ₃ → ClO + NO ₂	2	2.4 × 10 ⁻¹¹		Mellouki et al. (1987)
Cl 7	Cl + CH ₄ $\xrightarrow{O_2}$ HCl + CH ₃ OO	2	9.6 × 10 ⁻¹²	-1360	Sander et al. (2003)
Cl 8	Cl + C ₂ H ₆ $\xrightarrow{O_2}$ HCl + C ₂ H ₅ O ₂	2	7.7 × 10 ⁻¹¹	-90	Sander et al. (2003)
Cl 9	Cl + C ₂ H ₄ $\xrightarrow{O_2}$ HCl + C ₂ H ₅ O ₂	2	1. × 10 ⁻¹⁰		Sander et al. (1997), see note
Cl 10	Cl + HCHO $\xrightarrow{O_2}$ HCl + HO ₂ + CO	2	8.1 × 10 ⁻¹¹	-30	Sander et al. (2003)
Cl 11	Cl + ROOH → CH ₃ OO + HCl	2	5.7 × 10 ⁻¹¹		Wallington et al. (1990), see note
Cl 12	Cl + OClO → ClO + ClO	2	3.2 × 10 ⁻¹¹	170	Atkinson et al. (2006)
Cl 13	Cl + ClNO ₃ → Cl ₂ + NO ₃	2	6.5 × 10 ⁻¹²	135	Sander et al. (2003)
Cl 14	Cl + PAN → HCl + HCHO + NO ₃	2	1.0 × 10 ⁻¹⁴		Tsalkani et al. (1988)
Cl 15	Cl + HNO ₃ → HCl + NO ₂	2	1.0 × 10 ⁻¹⁶		Wine et al. (1988)
Cl 16	Cl + RONO ₂ → HCl + NO ₂	2	7.7 × 10 ⁻¹¹		estimated from Muthuramu et al. (1994)
Cl 17	ClO + OH → Cl + HO ₂	2	7.4 × 10 ⁻¹²	-270	Sander et al. (2003)
Cl 18	ClO + OH → HCl + O ₂	2	6.0 × 10 ⁻¹³	-230	Sander et al. (2003)
Cl 19	ClO + HO ₂ → HOCl + O ₂	2	2.2 × 10 ⁻¹²	340	Atkinson et al. (2006)
Cl 20	ClO + CH ₃ OO → Cl + HCHO + HO ₂	2	3.3 × 10 ⁻¹²	-115	Sander et al. (2003)
Cl 21	ClO + NO → Cl + NO ₂	2	6.2 × 10 ⁻¹²	295	Atkinson et al. (2006)
Cl 22	ClO + NO ₂ \xrightarrow{M} ClNO ₃	3	2		Atkinson et al. (2006)
Cl 23	ClO + ClO → Cl ₂ O ₂	2	2		Atkinson et al. (2006)
Cl 24	ClO + ClO → Cl ₂ + O ₂	2	1.0 × 10 ⁻¹²	-1590	Atkinson et al. (2006)
Cl 25	ClO + ClO → Cl ₂ O ₂	2	3.0 × 10 ⁻¹¹	-2450	Atkinson et al. (2006)
Cl 26	ClO + ClO → Cl + OClO	2	3.5 × 10 ⁻¹³	-1370	Atkinson et al. (2006)
Cl 27	OCIO + OH → HOCl + O ₂	2	4.5 × 10 ⁻¹³	800	Atkinson et al. (2006)
Cl 28	OCIO + NO → ClO + NO ₂	2	1.1 × 10 ⁻¹³	350	Atkinson et al. (2006)
Cl 29	Cl ₂ O ₂ → ClO + ClO	1	2		Atkinson et al. (2006)
Cl 30	HOCl + OH → ClO + H ₂ O	2	3.0 × 10 ⁻¹²	-500	Sander et al. (2003)
Cl 31	HCl + OH → H ₂ O + Cl	2	1.8 × 10 ⁻¹²	-240	Atkinson et al. (2006)
Cl 32	ClNO ₂ + OH → HOCl + NO ₂	2	2.4 × 10 ⁻¹²	-1250	Atkinson et al. (2006)

Table 2: Continued.

no	reaction	n	$A [(\text{cm}^{-3})^{1-n} \text{s}^{-1}]$	$-E_a / R [\text{K}]$	reference
Cl 33	$\text{ClNO}_3 + \text{OH} \longrightarrow 0.5 \text{ClO} + 0.5 \text{HNO}_3 + 0.5 \text{HOCl} + 0.5 \text{NO}_3$	2	1.2×10^{-12}	-330	Atkinson et al. (2006)
Cl 34	$\text{ClNO}_3 \longrightarrow \text{ClO} + \text{NO}_2$	1	2		Anderson and Fahey (1990)
Cl 35	$\text{OCIO} + h\nu \xrightarrow{\text{O}_2, \text{O}_3} \text{O}_3 + \text{ClO}$	1	1		DeMore et al. (1997)
Cl 36	$\text{Cl}_2\text{O}_2 + h\nu \longrightarrow \text{Cl} + \text{Cl} + \text{O}_2$	1	1		DeMore et al. (1997)
Cl 37	$\text{Cl}_2 + h\nu \longrightarrow 2 \text{Cl}$	1	1		DeMore et al. (1997)
Cl 38	$\text{HOCl} + h\nu \longrightarrow \text{Cl} + \text{OH}$	1	1		DeMore et al. (1997)
Cl 39	$\text{ClNO}_2 + h\nu \longrightarrow \text{Cl} + \text{NO}_2$	1	1		DeMore et al. (1997)
Cl 40	$\text{ClNO}_3 + h\nu \longrightarrow \text{Cl} + \text{NO}_3$	1	1		DeMore et al. (1997)
Br 1	$\text{Br} + \text{O}_3 \longrightarrow \text{BrO} + \text{O}_2$	2	1.7×10^{-11}	-800	Atkinson et al. (2006)
Br 2	$\text{Br} + \text{HO}_2 \longrightarrow \text{HBr} + \text{O}_2$	2	7.7×10^{-12}	-450	Atkinson et al. (2006)
Br 3	$\text{Br} + \text{C}_2\text{H}_4 \xrightarrow{\text{O}_2} \text{HBr} + \text{C}_2\text{H}_5\text{O}_2$	2	$5. \times 10^{-14}$		Sander et al. (1997), see note
Br 4	$\text{Br} + \text{HCHO} \xrightarrow{\text{O}_2} \text{HBr} + \text{CO} + \text{HO}_2$	2	1.7×10^{-11}	-800	Sander et al. (2003)
Br 5	$\text{Br} + \text{ROOH} \longrightarrow \text{CH}_3\text{OO} + \text{HBr}$	2	2.66×10^{-12}	-1610	Mallard et al. (1993), see note
Br 6	$\text{Br} + \text{NO}_2 \longrightarrow \text{BrNO}_2$	2	2		Sander et al. (2003)
Br 7	$\text{Br} + \text{BrNO}_3 \longrightarrow \text{Br}_2 + \text{NO}_3$	2	4.9×10^{-11}		Orlando and Tyndall (1996)
Br 8	$\text{BrO} + \text{OH} \longrightarrow \text{Br} + \text{HO}_2$	2	1.8×10^{-11}	250	Atkinson et al. (2006)
Br 9	$\text{BrO} + \text{HO}_2 \longrightarrow \text{HOBr} + \text{O}_2$	2	4.5×10^{-12}	500	Atkinson et al. (2006)
Br 10	$\text{BrO} + \text{CH}_3\text{OO} \longrightarrow \text{HOBr} + \text{HCHO}$	2	4.1×10^{-12}		Aranda et al. (1997)
Br 11	$\text{BrO} + \text{CH}_3\text{OO} \longrightarrow \text{Br} + \text{HCHO} + \text{HO}_2$	2	1.6×10^{-12}		Aranda et al. (1997)
Br 12	$\text{BrO} + \text{HCHO} \xrightarrow{\text{O}_2} \text{HOBr} + \text{CO} + \text{HO}_2$	2	1.5×10^{-14}		Hansen et al. (1999)
Br 13	$\text{BrO} + \text{NO} \longrightarrow \text{Br} + \text{NO}_2$	2	8.7×10^{-12}	260	Atkinson et al. (2006)
Br 14	$\text{BrO} + \text{NO}_2 \xrightarrow{M} \text{BrNO}_3$	3	2		Atkinson et al. (2006)
Br 15	$\text{BrO} + \text{BrO} \longrightarrow 2 \text{Br} + \text{O}_2$	2	2.4×10^{-12}	40	Sander et al. (2003)
Br 16	$\text{BrO} + \text{BrO} \longrightarrow \text{Br}_2 + \text{O}_2$	2	2.9×10^{-14}	860	Sander et al. (2003)
Br 17	$\text{HBr} + \text{OH} \longrightarrow \text{Br} + \text{H}_2\text{O}$	2	5.5×10^{-12}	205	Atkinson et al. (2006)
Br 18	$\text{BrNO}_3 \longrightarrow \text{BrO} + \text{NO}_2$	1	2		Orlando and Tyndall (1996)
Br 19	$\text{BrO} + h\nu \xrightarrow{\text{O}_2} \text{Br} + \text{O}_3$	1	1		DeMore et al. (1997)
Br 20	$\text{Br}_2 + h\nu \longrightarrow 2 \text{Br}$	1	1		Hubinger and Nee (1995)
Br 21	$\text{HOBr} + h\nu \longrightarrow \text{Br} + \text{OH}$	1	1		Ingham et al. (1999)
Br 22	$\text{BrNO}_2 + h\nu \longrightarrow \text{Br} + \text{NO}_2$	1	1		Scheffer et al. (1997)
Br 23	$\text{BrNO}_3 + h\nu \longrightarrow \text{Br} + \text{NO}_3$	1	1		DeMore et al. (1997)
Br 24	$\text{Br}_2 + \text{OH} \longrightarrow \text{HOBr} + \text{Br}$	1	1		Atkinson et al. (2006)
Br 25	$\text{CH}_3\text{Br} + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{Br}$	2	2.0×10^{-11}	240	Atkinson et al. (2006)
Br 26	$\text{CHBr}_3 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{Br}$	2	1.7×10^{-12}	-1215	Atkinson et al. (2006)
		2	1.35×10^{-12}	-600	Atkinson et al. (2004)

Table 2: Continued.

no	reaction	n	A [(cm ³) ¹⁻ⁿ s ⁻¹]	$-E_a / R$ [K]	reference
Hx 1	Cl + BrCl → Br + Cl ₂	2	1.5 × 10 ⁻¹¹		Mallard et al. (1993)
Hx 2	Cl + Br ₂ → BrCl + Br	2	1.2 × 10 ⁻¹⁰		Mallard et al. (1993)
Hx 3	Br + OClO → BrO + ClO	2	2.6 × 10 ⁻¹¹	-1300	Atkinson et al. (2006)
Hx 4	Br + Cl ₂ → BrCl + Cl	2	1.1 × 10 ⁻¹⁵		Mallard et al. (1993)
Hx 5	Br + BrCl → Br ₂ + Cl	2	3.3 × 10 ⁻¹⁵		Mallard et al. (1993)
Hx 6	BrO + ClO → Br + OClO	2	1.6 × 10 ⁻¹²	430	Atkinson et al. (2006)
Hx 7	BrO + ClO → Br + Cl + O ₂	2	2.9 × 10 ⁻¹²	220	Atkinson et al. (2006)
Hx 8	BrO + ClO → BrCl + O ₂	2	5.8 × 10 ⁻¹³	170	Atkinson et al. (2006)
Hx 9	BrCl + hν → 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). Notes: The rates for ROOH were assumed as that of CH₃OOH; C₂H₄ 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	$O_3 + OH \rightarrow HO_2$	2	1.1×10^8		Sehested et al. (1984)
O 2	$O_3 + O_2^- \rightarrow OH + OH^-$	2	1.5×10^9		Sehested et al. (1983)
O 3	$OH + OH \rightarrow H_2O_2$	2	5.5×10^9		Buxton et al. (1988)
O 4	$OH + HO_2 \rightarrow H_2O$	2	7.1×10^9		Sehested et al. (1968)
O 5	$OH + O_2^- \rightarrow OH^-$	2	1.0×10^{10}		Sehested et al. (1968)
O 6	$OH + H_2O_2 \rightarrow HO_2$	2	2.7×10^7	-1684	Christensen et al. (1982)
O 7	$HO_2 + HO_2 \rightarrow H_2O_2$	2	9.7×10^5	-2500	Christensen and Sehested (1988)
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	1.0×10^8	-900	Christensen and Sehested (1988)
N 1	$HONO + OH \rightarrow NO_2$	2	1.0×10^{10}		assumed =N7 Barker et al. (1970)
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3$	3	4.6×10^3	-6800	Damschen and Martin (1983)
N 3	$NO_3 + OH^- \rightarrow NO_3^- + OH$	2	8.2×10^7	-2700	Exner et al. (1992)
N 4	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	2	1.0×10^8		Lee and Schwartz (1981)
N 5	$NO_2 + HO_2 \rightarrow HNO_4$	2	1.8×10^9		Warneck (1999)
N 6	$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	2	5.0×10^5	-6950	Damschen and Martin (1983)
N 7	$NO_2^- + OH \rightarrow NO_2 + OH^-$	2	1.0×10^{10}		Barker et al. (1970)
N 8	$NO_4^- \rightarrow NO_2^- + O_2$	1	8.0×10^{-1}		Warneck (1999)
C 1	$HCHO + OH \rightarrow HCOOH + HO_2$	2	7.7×10^8	-1020	Chin and Wine (1994)
C 2	$HCOOH + OH \rightarrow HO_2 + CO_2$	2	1.1×10^8	-991	Chin and Wine (1994)
C 3	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	2	3.1×10^9	-1240	Chin and Wine (1994)
C 4	$CH_3OO + HO_2 \rightarrow CH_3OOH$	2	4.3×10^5		estimated by Jacob (1986)
C 5	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	2	5.0×10^7		estimated by Jacob (1986)
C 6	$CH_3OH + OH \rightarrow HCHO + HO_2$	2	9.7×10^8		Buxton et al. (1988)
C 7	$CH_3OOH + OH \rightarrow CH_3OO$	2	2.7×10^7	-1715	estimated by Jacob (1986)
C 8	$CH_3OOH + OH \rightarrow HCHO + OH$	2	1.1×10^7	-1715	estimated by Jacob (1986)
C 9	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	2	6.5×10^8		Ross et al. (1992)
C 10	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	2	4.3×10^5		Ross et al. (1992)
C 11	$CO_3^- + HCOO^- \rightarrow HCO_3^- + HCO_3^- + HO_2$	2	1.5×10^5		Ross et al. (1992)
C 12	$HCO_3^- + OH \rightarrow CO_3^-$	2	8.5×10^6		Ross et al. (1992)
C 13	$DOM + OH \rightarrow HO_2$	2	5.0×10^9		estimated by (C. Anastasio, pers. comm.) from Ross et al. (1998)

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a / R$ [K]	reference
S 1	$SO_3^- + O_2 \rightarrow SO_5^-$	2	1.5×10^9		Huie and Neta (1987)
S 2	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+ + O_2$	2	3.7×10^5	-5500	Hoffmann (1986)
S 3	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	2	1.5×10^9	-5300	Hoffmann (1986)
S 4	$HSO_3^- + OH \rightarrow SO_3^-$	2	4.5×10^9		Buxton et al. (1988)
S 5	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	2	5.5×10^9		Buxton et al. (1988)
S 6	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	2	3.0×10^3		upper limit D. Sedlak pers. comm. with R. Sander
S 7	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	2	3.0×10^3		upper limit D. Sedlak pers. comm. with R. Sander
S 8	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	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	2.0×10^7		Clifton et al. (1988)
S 10	$SO_3^{2-} + NO_2 \xrightarrow{NO_2} SO_4^{2-} + HONO + HONO$	2	2.0×10^7		Clifton et al. (1988)
S 11	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	2	1.4×10^9	-2000	Exner et al. (1992)
S 12	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	2	3.1×10^5		Warneck (1999)
S 13	$HSO_3^- + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + H^+ + CH_3OH$	3	1.6×10^7	-3800	Lind et al. (1987)
S 14	$SO_3^{2-} + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + CH_3OH$	3	1.6×10^7	-3800	Lind et al. (1987)
S 15	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	2	4.3×10^{-1}		Boyce and Hoffmann (1984)
S 16	$SO_3^{2-} + HCHO \xrightarrow{H^+} CH_2OHSO_3^-$	2	1.4×10^4		Boyce and Hoffmann (1984)
S 17	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	2	3.6×10^3		Seinfeld and Pandis (1998)
S 18	$HSO_3^- + HSO_5^- \xrightarrow{H^+} SO_4^{2-} + SO_4^{2-} + H^+ + H^+$	3	7.1×10^6		Betterton and Hoffmann (1988)
S 19	$SO_4^- + OH \rightarrow HSO_5^-$	2	1.0×10^9		Jiang et al. (1992)

Table 3: Continued.

no	reaction	n	k_0 [$(M^{1-n})s^{-1}$]	$-E_a / R$ [K]	reference
S 20	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	2	3.5×10^9		Jiang et al. (1992)
S 21	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	2	3.5×10^9		assumed =S20
S 22	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	2	1.1×10^{11}	-1110	Herrmann et al. (1995)
S 23	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	2	1.2×10^7		Wine et al. (1989)
S 24	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	2	5.0×10^4		Exner et al. (1992)
S 25	$SO_4^- + HSO_3^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	2	8.0×10^8		Huie and Neta (1987)
S 26	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	2	4.6×10^8		Huie and Neta (1987)
S 27	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	2	1.0×10^5		Logager et al. (1993)
S 28	$SO_5^- + HSO_3^- \rightarrow SO_4^- + SO_4^{2-} + H^+$	2	7.5×10^4		Huie and Neta (1987)
S 29	$SO_5^- + SO_3^{2-} \rightarrow SO_4^- + SO_4^{2-}$	2	9.4×10^6		Huie and Neta (1987)
S 30	$SO_5^- + HSO_3^- \rightarrow SO_3^- + HSO_5^-$	2	2.5×10^4		Huie and Neta (1987); Deister and Warneck (1990)
S 31	$SO_5^- + SO_3^{2-} \xrightarrow{H^+} SO_3^- + HSO_5^-$	2	3.6×10^6		Huie and Neta (1987); Deister and Warneck (1990)
S 32	$SO_5^- + O_2^- \xrightarrow{H^+} HSO_5^- + O_2$	2	2.3×10^8		Buxton et al. (1996)
S 33	$SO_5^- + SO_5^- \rightarrow H_2O$	2	1.0×10^8		Ross et al. (1992)
S 34	$DMS + O_3 \rightarrow O_2 + DMSO$	2	8.6×10^8	-2600	Gershenzon et al. (2001)
S 35	$DMS + OH \rightarrow 0.5 CH_3SO_3^- + 0.5 CH_3OO + 0.5 HSO_4^- + HCHO + H^+$	2	1.9×10^{10}		Ross et al. (1998)
S 36	$DMSO + OH \rightarrow CH_3SO_2^- + CH_3OO + H^+$	2	4.5×10^9		Bardouki et al. (2002)
S 37	$CH_3SO_2^- + OH \rightarrow CH_3SO_3^- + H_2O - O_2$	2	1.2×10^{10}		Bardouki et al. (2002)
S 38	$CH_3SO_3^- + OH \rightarrow SO_4^{2-} + H^+ + CH_3OO$	2	1.2×10^7		Bonsang et al. (1991)

Table 3: Continued.

no	reaction	n	k_0 [(M ¹⁻ⁿ)s ⁻¹]	$-E_a / R$ [K]	reference
Cl 1	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl}^- + \text{H}^+$	2	2.0×10^9		Yu (2001)
Cl 2	$\text{Cl} + \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{ClOH}^-$	2	1.8×10^5		Yu (2001)
Cl 3	$\text{Cl} + \text{NO}_3^- \rightarrow \text{NO}_3 + \text{Cl}^-$	2	1.0×10^8		Buxton et al. (1999b)
Cl 4	$\text{Cl} + \text{DOM} \rightarrow \text{Cl}^- + \text{HO}_2$	2	5.0×10^9		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Cl 5	$\text{Cl} + \text{SO}_4^{2-} \rightarrow \text{SO}_4^- + \text{Cl}^-$	2	2.1×10^8		Buxton et al. (1999a)
Cl 6	$\text{Cl} + \text{Cl} \rightarrow \text{Cl}_2$	2	8.8×10^7		Wu et al. (1980)
Cl 7	$\text{Cl}^- + \text{OH} \rightarrow \text{ClOH}^-$	2	4.2×10^9		Yu (2001)
Cl 8	$\text{Cl}^- + \text{O}_3 \rightarrow \text{ClO}^- + \text{O}_2$	2	3.0×10^{-3}		Hoigné et al. (1985)
Cl 9	$\text{Cl}^- + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{Cl}$	2	9.3×10^6	-4330	Exner et al. (1992)
Cl 10	$\text{Cl}^- + \text{SO}_4^- \rightarrow \text{SO}_4^{2-} + \text{Cl}$	2	2.5×10^8		Buxton et al. (1999a)
Cl 11	$\text{Cl}^- + \text{HSO}_5^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	2	1.8×10^{-3}	-7352	Fortnum et al. (1960)
Cl 12	$\text{Cl}^- + \text{HOCl} + \text{H}^+ \rightarrow \text{Cl}_2$	3	2.2×10^4	-3508	Ayers et al. (1996)
Cl 13	$\text{Cl}_2 \rightarrow \text{Cl}^- + \text{HOCl} + \text{H}^+$	1	2.2×10^1	-8012	Ayers et al. (1996)
Cl 14	$\text{Cl}_2^- + \text{OH} \rightarrow \text{HOCl} + \text{Cl}^-$	2	1.0×10^9		Ross et al. (1998)
Cl 15	$\text{Cl}_2^- + \text{OH}^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{OH}$	2	4.0×10^6		Jacobi (1996)
Cl 16	$\text{Cl}_2^- + \text{HO}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{O}_2$	2	3.1×10^9		Yu (2001)
Cl 17	$\text{Cl}_2^- + \text{O}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{O}_2$	2	6.0×10^9		Jacobi (1996)
Cl 18	$\text{Cl}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{HO}_2$	2	7.0×10^5	-3340	Jacobi (1996)
Cl 19	$\text{Cl}_2^- + \text{NO}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{NO}_2$	2	6.0×10^7		Jacobi (1996)
Cl 20	$\text{Cl}_2^- + \text{CH}_3\text{OOH} \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{CH}_3\text{OO}$	2	7.0×10^5	-3340	Jacobi (1996)
Cl 21	$\text{Cl}_2^- + \text{DOM} \rightarrow \text{Cl}^- + \text{Cl}^- + \text{HO}_2$	2	1.0×10^6		assumed by Jacobi (1996) estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Cl 22	$\text{Cl}_2^- + \text{HSO}_3^- \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^- + \text{H}^+$	2	4.7×10^8	-1082	Shoute et al. (1991)
Cl 23	$\text{Cl}_2^- + \text{SO}_3^{2-} \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^-$	2	6.2×10^7		Jacobi et al. (1996)
Cl 24	$\text{Cl}_2^- + \text{Cl}_2^- \rightarrow \text{Cl}_2 + 2\text{Cl}^-$	2	6.2×10^9		Yu (2001)
Cl 25	$\text{Cl}_2^- + \text{Cl}^- \rightarrow \text{Cl}^- + \text{Cl}_2$	2	2.7×10^9		Yu (2001)
Cl 26	$\text{Cl}_2^- + \text{DMS} \rightarrow 0.5 \text{CH}_3\text{SO}_3^- + 0.5 \text{CH}_3\text{OO} + 0.5 \text{HSO}_4^- + \text{HCHO} + 2 \text{Cl}^- + 2 \text{H}^+$	2	3.0×10^9		rate from Ross et al. (1998)
Cl 27	$\text{ClOH}^- \rightarrow \text{Cl}^- + \text{OH}$	1	6.0×10^9		Yu (2001)
Cl 28	$\text{ClOH}^- + \text{H}^+ \rightarrow \text{Cl}$	2	4.0×10^{10}		Yu (2001)
Cl 29	$\text{HOCl} + \text{HO}_2 \rightarrow \text{Cl} + \text{O}_2$	2	7.5×10^6		assumed = Cl30 Long and Bielski (1980)
Cl 30	$\text{HOCl} + \text{O}_2^- \rightarrow \text{Cl} + \text{OH}^- + \text{O}_2$	2	7.5×10^6		Long and Bielski (1980)
Cl 31	$\text{HOCl} + \text{SO}_3^{2-} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	2	7.6×10^8		Fogelman et al. (1989)
Cl 32	$\text{HOCl} + \text{HSO}_3^- \rightarrow \text{Cl}^- + \text{HSO}_4^- + \text{H}^+$	2	7.6×10^8		assumed = Cl31 Fogelman et al. (1989)
Cl 33	$\text{Cl}_2 + \text{HO}_2 \rightarrow \text{Cl}_2^- + \text{H}^+ + \text{O}_2$	2	1.0×10^9		Bjergbakke et al. (1981)
Cl 34	$\text{Cl}_2 + \text{O}_2^- \rightarrow \text{Cl}_2^- + \text{O}_2$	2	1.0×10^9		assumed = Cl33 Bjergbakke et al. (1981)
Cl 35	$\text{Cl}^- + \text{HNO}_4 \rightarrow \text{HOCl} + \text{NO}_3^-$	2	1.4×10^{-2}		Régimbal and Mozurkewich (1997)

Table 3: Continued.

no	reaction	n	k_0 [(M ¹⁻ⁿ)s ⁻¹]	$-E_a / R$ [K]	reference
Br 1	$\text{Br} + \text{OH}^- \rightarrow \text{BrOH}^-$	2	1.3×10^{10}		Zehavi and Rabani (1972)
Br 2	$\text{Br} + \text{DOM} \rightarrow \text{Br}^- + \text{HO}_2$	2	2.0×10^8		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Br 3	$\text{Br}^- + \text{OH} \rightarrow \text{BrOH}^-$	2	1.1×10^{10}		Zehavi and Rabani (1972)
Br 4	$\text{Br}^- + \text{O}_3 \rightarrow \text{BrO}^-$	2	2.1×10^2	-4450	Haag and Hoigné (1983)
Br 5	$\text{Br}^- + \text{NO}_3 \rightarrow \text{Br} + \text{NO}_3^-$	2	3.8×10^9		Zellner et al. 1996 in Herrmann et al. (2000)
Br 6	$\text{Br}^- + \text{SO}_4^- \rightarrow \text{Br} + \text{SO}_4^{2-}$	2	2.1×10^9		Jacobi (1996)
Br 7	$\text{Br}^- + \text{HSO}_5^- \rightarrow \text{HOBr} + \text{SO}_4^{2-}$	2	1.0	-5338	Fortnum et al. (1960)
Br 8	$\text{Br}^- + \text{HOBr} + \text{H}^+ \rightarrow \text{Br}_2$	3	1.6×10^{10}		Liu and Margerum (2001)
Br 9	$\text{Br}_2 \rightarrow \text{Br}^- + \text{HOBr} + \text{H}^+$	1	9.7×10^1	7457	Liu and Margerum (2001)
Br 10	$\text{Br}_2^- + \text{O}_2^- \rightarrow \text{Br}^- + \text{Br}^-$	2	1.7×10^8		Wagner and Strehlow (1987)
Br 11	$\text{Br}_2^- + \text{HO}_2 \rightarrow \text{Br}_2 + \text{H}_2\text{O}_2 - \text{H}^+$	2	4.4×10^9		Matthew et al. (2003)
Br 12	$\text{Br}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{HO}_2$	2	5.0×10^2		Chameides and Stelson (1992)
Br 13	$\text{Br}_2^- + \text{Br}_2 \rightarrow \text{Br}^- + \text{Br}^- + \text{Br}_2$	2	1.9×10^9		Ross et al. (1992)
Br 14	$\text{Br}_2^- + \text{CH}_3\text{OOH} \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{CH}_3\text{OO}$	2	1.0×10^5		assumed by Jacobi (1996)
Br 15	$\text{Br}_2^- + \text{DOM} \rightarrow \text{Br}^- + \text{Br}^- + \text{HO}_2$	2	1.0×10^5		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Br 16	$\text{Br}_2^- + \text{NO}_2^- \rightarrow \text{Br}^- + \text{Br}^- + \text{NO}_2$	2	1.7×10^7	-1720	Shoute et al. (1991)
Br 17	$\text{Br}_2^- + \text{HSO}_3^- \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{SO}_3^-$	2	6.3×10^7	-782	Shoute et al. (1991)
Br 18	$\text{Br}_2^- + \text{SO}_3^{2-} \rightarrow \text{Br}^- + \text{Br}^- + \text{SO}_3^-$	2	2.2×10^8	-650	Shoute et al. (1991)
Br 19	$\text{Br}_2^- + \text{DMS} \rightarrow 0.5 \text{CH}_3\text{SO}_3^- + 0.5 \text{CH}_3\text{OO} + 0.5 \text{HSO}_4^- + \text{HCHO} + 2 \text{H}^+$	2	3.2×10^9		rate from Ross et al. (1998)
Br 20	$\text{BrOH}^- \rightarrow \text{Br}^- + \text{OH}$	1	3.3×10^7		Zehavi and Rabani (1972)
Br 21	$\text{BrOH}^- \rightarrow \text{Br} + \text{OH}^-$	1	4.2×10^6		Zehavi and Rabani (1972)
Br 22	$\text{BrOH}^- + \text{H}^+ \rightarrow \text{Br}$	2	4.4×10^{10}		Zehavi and Rabani (1972)
Br 23	$\text{BrOH}^- + \text{Br}^- \rightarrow \text{Br}_2^- + \text{OH}^-$	2	1.9×10^8		Zehavi and Rabani (1972)
Br 24	$\text{BrO}^- + \text{SO}_3^{2-} \rightarrow \text{Br}^- + \text{SO}_4^{2-}$	2	1.0×10^8		Troy and Margerum (1991)
Br 25	$\text{HOBr} + \text{HO}_2 \rightarrow \text{Br} + \text{O}_2$	2	1.0×10^9		Herrmann et al. (1999)
Br 26	$\text{HOBr} + \text{O}_2^- \rightarrow \text{Br} + \text{OH}^- + \text{O}_2$	2	3.5×10^9		Schwarz and Bielski (1986)
Br 27	$\text{HOBr} + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{H}^+ + \text{O}_2$	2	1.2×10^6		von Gunten and Oliveras (1998)
Br 28	$\text{HOBr} + \text{SO}_3^- \rightarrow \text{Br}^- + \text{HSO}_4^-$	2	5.0×10^9		Troy and Margerum (1991)
Br 29	$\text{HOBr} + \text{HSO}_3^- \rightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$	2	5.0×10^9		assumed = Br28
Br 30	$\text{Br}_2 + \text{HO}_2 \rightarrow \text{Br}_2^- + \text{H}^+ + \text{O}_2$	2	1.1×10^8		Ross et al. (1998)
Br 31	$\text{Br}_2 + \text{O}_2^- \rightarrow \text{Br}_2^- + \text{O}_2$	2	5.6×10^9		Ross et al. (1998)
Br 32	$\text{Br}^- + \text{HNO}_4 \rightarrow \text{HOBr} + \text{NO}_3^-$	2	5.4×10^{-1}		Régimbal and Mozurkewich (1997)
Br 33	$\text{Br}^- + \text{O}_3 + \text{H}^+ \rightarrow \text{HOBr} + \text{O}_2$	3	11.7		Haag and Hoigné (1983)

Table 3: Continued.

no	reaction	n	k_0 [(M ¹⁻ⁿ)s ⁻¹]	$-E_a / R$ [K]	reference
Hx 1	Br ⁻ + HOCl + H ⁺ → BrCl	3	1.3 x 10 ⁶		Liu and Margerum (2001)
Hx 2	Cl ⁻ + HOBr + H ⁺ → BrCl	3	2.3 x 10 ¹⁰		Liu and Margerum (2001)
Hx 3	BrCl → Cl ⁻ + HOBr + H ⁺	1	3.0 x 10 ⁶		Liu and Margerum (2001)
Hx 4	Br ⁻ + ClO ⁻ + H ⁺ → BrCl + OH ⁻	3	3.7 x 10 ¹⁰		Kumar and Margerum (1987)
Hx 5	Cl ₂ + Br ⁻ → BrCl ₂ ⁻	2	7.7 x 10 ⁹		Liu and Margerum (2001)
Hx 6	BrCl ₂ ⁻ → Cl ₂ + Br ⁻	1	1.83 x 10 ³		Liu and Margerum (2001)
hv 1	O ₃ + hv → OH + OH + O ₂	1	1		assumed 2x gas phase
hv 2	H ₂ O ₂ + hv → 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 → OH + Cl	1	1		assumed 2x gas phase
hv 6	Cl ₂ + hv → Cl + Cl	1	1		assumed 2x gas phase
hv 7	HOBr + hv → OH + Br	1	1		assumed 2x gas phase
hv 8	Br ₂ + hv → Br + Br	1	1		assumed 2x gas phase
hv 9	BrCl + hv → 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	$\text{N}_2\text{O}_5 \xrightarrow{\text{H}_2\text{O}} \text{HNO}_{3aq} + \text{HNO}_{3aq}$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	Behnke et al. (1994), Behnke et al. (1997)
H 2	$\text{N}_2\text{O}_5 \xrightarrow{\text{Cl}^-} \text{ClNO}_2 + \text{NO}_3^-$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}f(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	Behnke et al. (1994), Behnke et al. (1997)
H 3	$\text{N}_2\text{O}_5 \xrightarrow{\text{Br}^-} \text{BrNO}_2 + \text{NO}_3^-$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}f(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	Behnke et al. (1994), Behnke et al. (1997)
H 4	$\text{ClNO}_3 \xrightarrow{\text{H}_2\text{O}} \text{HOCl}_{aq} + \text{HNO}_{3aq}$	$\bar{k}_t(\text{ClNO}_3)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	see note
H 5	$\text{ClNO}_3 \xrightarrow{\text{Cl}^-} \text{Cl}_{2aq} + \text{NO}_3^-$	$\bar{k}_t(\text{ClNO}_3)w_{l,i}f(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	see note
H 6	$\text{ClNO}_3 \xrightarrow{\text{Br}^-} \text{BrCl}_{aq} + \text{NO}_3^-$	$\bar{k}_t(\text{ClNO}_3)w_{l,i}f(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	see note
H 7	$\text{BrNO}_3 \xrightarrow{\text{H}_2\text{O}} \text{HOBr}_{aq} + \text{HNO}_{3aq}$	$\bar{k}_t(\text{BrNO}_3)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	see note
H 8	$\text{BrNO}_3 \xrightarrow{\text{Cl}^-} \text{BrCl}_{aq} + \text{NO}_3^-$	$\bar{k}_t(\text{BrNO}_3)w_{l,i}f(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	see note
H 9	$\text{BrNO}_3 \xrightarrow{\text{Br}^-} \text{Br}_{2aq} + \text{NO}_3^-$	$\bar{k}_t(\text{BrNO}_3)w_{l,i}f(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	see note

For a definition of \bar{k}_t and $w_{l,i}$ see von Glasow et al. (2002) or von Glasow (2000). $\text{Het}_T = [\text{H}_2\text{O} + f(\text{Cl}^-)[\text{Cl}^-] + f(\text{Br}^-)[\text{Br}^-]]$, with $f(\text{Cl}^-) = 5.0 \times 10^2$ and $f(\text{Br}^-) = 3.0 \times 10^5$. H4 - H9: the total rate is determined by \bar{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	$\text{CO}_{2aq} \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	1	2	4.3×10^{-7}	-913	Chameides (1984)
EQ 2	$\text{NH}_{3aq} \rightleftharpoons \text{OH}^- + \text{NH}_4^+$	1	2	1.7×10^{-5}	-4325	Chameides (1984)
EQ 3	$\text{H}_2\text{O}_{aq} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1	2	1.0×10^{-14}	-6716	Chameides (1984)
EQ 4	$\text{HCOOH}_{aq} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1	2	1.8×10^{-4}		Weast (1980)
EQ 5	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	1	2	6.0×10^{-8}	1120	Chameides (1984)
EQ 6	$\text{H}_2\text{SO}_{4aq} \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1	2	1.0×10^3		Seinfeld and Pandis (1998)
EQ 7	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1	2	1.2×10^{-2}	1120	Weast (1980)
EQ 8	$\text{HO}_{2aq} \rightleftharpoons \text{O}_2^- + \text{H}^+$	1	2	1.6×10^{-5}		Weinstein-Lloyd and Schwartz (1991)
EQ 9	$\text{SO}_{2aq} \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1	2	1.7×10^{-2}	2090	Chameides (1984)
EQ 10	$\text{Cl}_2 \rightleftharpoons \text{Cl}_{aq} + \text{Cl}^-$	1	2	5.2×10^{-6}		Jayson et al. (1973)
EQ 11	$\text{HOCl}_{aq} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	1	2	3.2×10^{-8}		Lax (1969)
EQ 12	$\text{HBr}_{aq} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1	2	1.0×10^9		Lax (1969)
EQ 13	$\text{Br}_2 \rightleftharpoons \text{Br}_{aq} + \text{Br}^-$	1	2	9.1×10^{-6}		Mamou et al. (1977)
EQ 14	$\text{HOBr}_{aq} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	1	2	2.3×10^{-9}	-3091	Kelley and Tartar (1956)
EQ 15	$\text{BrCl}_{aq} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	2	1	3.8	1143	Wang et al. (1994)
EQ 16	$\text{BrCl}_{aq} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	2	1	1.8×10^4		Wang et al. (1994)
EQ 17	$\text{Br}_{2aq} + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	2	1	1.3		Wang et al. (1994)
EQ 18	$\text{HNO}_{3aq} \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	1	2	1.5×10^1		Davis and de Bruin (1964)
EQ 19	$\text{HCl}_{aq} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1	2	1.7×10^6		Marsh and McElroy (1985)
EQ 20	$\text{HONO}_{aq} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	1	2	5.1×10^{-4}	-1260	Schwartz and White (1981)
EQ 21	$\text{HNO}_{4aq} \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1	2	1.0×10^{-5}	8700	Warneck (1999)

The temperature dependence is $K = K_0 \times \exp\left(\frac{-\Delta H}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, $T_0 = 298$ 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 ₂ O 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)
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)
CH ₃ OO	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	DeMore et al. (1997)
SO ₂	1.2	3120	Chameides (1984)	0.11	0	Pöschl et al. (1998)
H ₂ SO ₄	∞	—	assumed	0.65	(at 303 K)	Lucas and Prinn (2002)
CH ₃ SO ₂ H	∞	—	assumed	0.0002	0	De Bruyn et al. (1994)
CH ₃ SO ₃ H	∞	—	assumed	0.076	1762	De Bruyn et al. (1994)

For ROOH the values of CH₃OOH 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 $dl n(\frac{\alpha}{1-\alpha})/d(\frac{1}{T}) = -\frac{\Delta_{obs}H}{R}$. RT stands for ‘‘room temperature’’.

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