

Table 1: Initial Concentrations for three scenarios under polluted continental (urban), unpolluted continental (remote) and marine conditions (gas phase species in [ppb], aqueous phase species in [M])

	urban		remote		marine	
gas phase species						
NO ₂	4.5	a	1.5	a	0.4	k
HNO ₃	1	b	0.3	b	0.15	g
CH ₄	1700	a	1700	a	1700	a
H ₂ O ₂	1	d	0.001	a	0.001	a
H ₂	2000	a	2000	a	2000	a
CO	200	a	150	a	140	a
O ₃	90	a	60	a	40	a
HCl	6	a	0.7	b	0.5	g
NH ₃	25	a	1.5	b	0.05	g
CO ₂	5 · 10 ⁵	a	3.3 · 10 ⁵	b	3.3 · 10 ⁵	b
SO ₂	10	h	1	h	0.1	h
HCHO	0.1	a	0.1	a	0.01	a
C ₂ H ₆	2	a	1.5	a	1	a
HC3: Alkanes with OH rate constant between 2.7 · 10 ⁻¹³ and 3.4 · 10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	2	a	1	a	1	a
HC5: Alkanes with OH rate constant between 3.4 · 10 ⁻¹² and 6.8 · 10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	1	a	0.5	a	0	a
HC8: Alkanes with OH rate constant greater than 6.8 · 10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	0.1	a	0	a	0	a
C ₂ H ₄	1	a	0.5	a	0.1	a
OLT: Terminal alkenes	0.1	a	0.1	a	0.1	a
Isoprene	0.1	a	0.1	a	0.1	a
TOL: Toluene and less reactive aromatics	0.1	a	0.01	a	0	a
CSL: Cresol and other OH-substituted aromatics	0.001	a	0.001	a	0	a
XYL: Xylene and more reactive aromatics	0.1	a	0.01	a	0	a
ALD: Acetaldehyde and higher aldehydes	0.1	a	0.1	a	0.01	a
Ketones	0.1	a	0.1	a	0.01	a
Glyoxal	0.1	a	0.1	a	0.01	a
Methylglyoxal	0.1	a	0.1	a	0.01	a
PAN	0.01	a	0.01	a	0.01	a
CH ₃ OOH	0.01	a	0.01	a	0.01	a
OP2: Higher organic peroxides	0.01	a	0.01	a	0.01	a
CH ₃ C(O)OOH	0.001	a	0.001	a	0.001	a
CH ₃ OH	5	a	2	f	0.8	g
EtOH	1	c	0.24	f	2.4 · 10 ⁻³	h

aqueous phase species

O _{2(aq)}	$3 \cdot 10^{-4}$	b	$3 \cdot 10^{-4}$	b	$3 \cdot 10^{-4}$	b
OH ⁻	$3.16 \cdot 10^{-10}$	b	$3.16 \cdot 10^{-10}$	b	$1.6 \cdot 10^{-9}$	b
pH	4.5	b	4.5	b	5.2	i
Cl ⁻	$1 \cdot 10^{-4}$	h	$1 \cdot 10^{-4}$	h	$5.6 \cdot 10^{-4}$	j
Br ⁻	$3 \cdot 10^{-6}$	h	$3 \cdot 10^{-7}$	h	$1.8 \cdot 10^{-6}$	j
Fe ³⁺	$5 \cdot 10^{-6}$	d	$5 \cdot 10^{-7}$	d	$5 \cdot 10^{-8}$	d
Mn ³⁺	$2.5 \cdot 10^{-7}$	d	$2.5 \cdot 10^{-8}$	d	$1 \cdot 10^{-9}$	d
Cu ⁺	$2.5 \cdot 10^{-7}$	d	$2.5 \cdot 10^{-8}$	d	$1 \cdot 10^{-9}$	d
HSO ₄ ⁻	$3 \cdot 10^{-7}$		$3 \cdot 10^{-7}$		$3 \cdot 10^{-8}$	
SO ₄ ²⁻	$5.97 \cdot 10^{-5}$	e	$5.97 \cdot 10^{-5}$	e	$5.97 \cdot 10^{-6}$	i

Constant concentrations

during the simulation time [ppb] or [M]:

H ₂ O _(g)	$2 \cdot 10^7$	$3 \cdot 10^7$	$3 \cdot 10^7$
O _{2(g)}	$2 \cdot 10^8$	$2 \cdot 10^8$	$2 \cdot 10^8$
N _{2(g)}	$7.8 \cdot 10^8$	$7.8 \cdot 10^8$	$7.8 \cdot 10^8$
H ₂ O _(aq)	55.5	55.5	55.5

^a Zimmermann and Poppe, 1996; ^b Graedel and Weschler, 1981; ^c Saxena and Hildemann, 1996; ^d Matthijssen and Bultjes, 1995; ^e Weschler et al., 1986; ^f Leibrock and Slemr, 1996; ^g Jacob, 1986; ^h estimated; ⁱ Chameides, 1984; ^j Herrmann *et al.*, 1996; ^k Rohrer and Brüning, 1992

Table 2: Uptake Parameters**Table 2a: Henry's law constants**

Reaction No.	Species	K_{H298} , M atm ⁻¹	ΔH_{298} , kJ mol ⁻¹	References
H1	CO ₂	$3.11 \cdot 10^{-2}$	-20.14	Chameides, 1984
H2	HCl	1.10	-16.8	Marsh and McElroy, 1985
H3	NH ₃	60.7	-32.6	Clegg and Brimblecombe, 1990
H4	O ₃	$1.14 \cdot 10^{-2}$	-19.1	Kosak-Channing and Helz, 1983
H5	HO ₂	$9 \cdot 10^3$		Weinstein-Lloyd and Schwartz, 1991
H6	OH	25	-43.9	Kläning et al., 1985 National Bureau of Standards, 1971
H7	H ₂ O ₂	$1.02 \cdot 10^5$	-52.7	Lind and Kok, 1994
H8	HNO ₃	$2.1 \cdot 10^5$	-72.3	Lelieveld and Crutzen, 1991
H9	NO ₃	0.6		Rudich <i>et al.</i> , 1996
H10	N ₂ O ₅	1.4		ⁱ
H11	NO ₂	$1.2 \cdot 10^{-2}$	-10.5	Schwartz and White, 1982
H12	HNO ₂	49	-40.6	Park and Lee, 1988
H13	HO ₂ NO ₂	$1 \cdot 10^{5d}$		$K_{H13} = K_{H7}$
H14	SO ₂	1.24	-27	Beilke and Gravenhorst, 1978
H15	HCHO ^a	$3.0 \cdot 10^3$	-60	Betterton and Hoffmann, 1988a
H16	CH ₃ OOH	6	-44.2	Lind and Kok, 1994
H17	CH ₃ C(O)OOH	$6.69 \cdot 10^2$	-49.0	Lind and Kok, 1994
H18	CH ₃ OH	$2.2 \cdot 10^2$	-44.8	Betterton, 1992
H19	C ₂ H ₅ OH	$1.9 \cdot 10^2$	-52.3	Betterton, 1992
H20	CH ₃ CHO ^b	11.4	-52	Betterton and Hoffmann, 1988a
H21	HCOOH	$5.53 \cdot 10^3$	-46.8	Khan and Brimblecombe, 1992
H22	CH ₃ COOH	$5.50 \cdot 10^3$	-49.0	Khan and Brimblecombe, 1992
H23	CH ₃ O ₂	6	-46.9	Jacob, 1986
H24	ETHP ^c	6 ^d	-46.9 ^d	$K_{H24} = K_{H23}$
H25	Cl ₂	$9.15 \cdot 10^{-2}$	20.7	Wilhelm <i>et al.</i> , 1977
H26	Br ₂	0.758	31.6	Loomis, 1928
H27	H ₂ SO ₄	$2.1 \cdot 10^5$		$K_{H27} = K_{H8}$
H28	CH ₄	$1.46 \cdot 10^{-3}$		Mackay and Shan, 1981
H29	C ₂ H ₆	$1.95 \cdot 10^{-3}$		Mackay and Shan, 1981
H30	C ₂ H ₄	$4.55 \cdot 10^{-3}$		Mackay and Shan, 1981
H31	PAN ^e	5		Holdren et al., 1984
H32	OP2 ^f	837		O'Sullivan et al., 1996
H33	OL2P ^g	6		$K_{H33} = K_{H23}$
H34	ACO ₃ ^h	669		$K_{H34} = K_{H17}$

^a Equilibrium HCHO (g) \leftrightarrow CH₂(OH)₂ (aq).; ^b Equilibrium CH₃CHO (g) \leftrightarrow CH₃CH(OH)₂ (aq).; ^c Peroxy radical with 2 carbon atoms.; ^d Estimated value.; ^e Peroxy acetyl nitrate ^f C₂-hydroperoxides; ^g Peroxy radicals of C₂H₄; ^h Acetyl peroxy radical; ⁱ estimated $K_{H(N2O5)} = K_{H(N2O4)}$ (Schwartz and White, 1983)

Table 2b: Mass accommodation coefficients and Gas Phase Diffusion Coefficients

Reaction No.	Species	α	References	D_g [$10^5 \text{ m}^2 \text{ s}^{-1}$]	References
H1	CO ₂	$2 \cdot 10^{-4}$	estimated	1.55	McElroy, 1997
H2	HCl	0.064	Davidovits <i>et al.</i> , 1995	1.89	Marsh and McElroy, 1985
H3	NH ₃	0.04	Bongartz, 1995	2.3	Ponche, 1993
H4	O ₃	0.05	Mirabel, 1996	1.48	Schwartz, 1986
H5	HO ₂	0.01	Hanson, 1992	1.04	Hanson, 1992
H6	OH	0.05	estimated	1.53	Hanson, 1992
H7	H ₂ O ₂	0.11	Davidovits <i>et al.</i> , 1995	1.46	McElroy, 1997
H8	HNO ₃	0.054	Davidovits <i>et al.</i> , 1995	1.32	Kirchner, 1990
H9	NO ₃	$4 \cdot 10^{-3}$	Kirchner, 1990 Rudich, 1996	1.00	Thomas, 1998
H10	N ₂ O ₅	$3.7 \cdot 10^{-3}$	George, 1986	1.10	Kirchner, 1990
H11	NO ₂	$1.5 \cdot 10^{-3}$	estimated	1.92	Ponche, 1993
H12	HNO ₂	0.5	Bongartz, 1995	1.30	Kirchner, 1990
H13	HO ₂ NO ₂	0.1	Jacob, 1986	1.30	Schweitzer, 1998
H14	SO ₂	$3.5 \cdot 10^{-2}$	Tang and Lee, 1987 Gardner, 1987	1.28	McElroy, 1997
H15	HCHO ^a	0.02	estimated	1.64	Fuller, 1986 ^{a)}
H16	CH ₃ OOH	$3.8 \cdot 10^{-3}$	Davidovits <i>et al.</i> , 1995	1.31	Fuller, 1986 ^{a)}
H17	CH ₃ C(O)OOH	0.019	$\alpha_{17} = \alpha_{31}$	1.02	Fuller, 1986 ^{a)}
H18	CH ₃ OH	$1.5 \cdot 10^{-2}$	Davidovits <i>et al.</i> , 1995	1.16	Schwartz, 1986
H19	C ₂ H ₅ OH	$8.2 \cdot 10^{-3}$	Davidovits <i>et al.</i> , 1995	0.95	Schwartz, 1986
H20	CH ₃ CHO ^b	0.03	estimated	1.22	Fuller, 1986 ^{a)}
H21	HCOOH	0.012	Davidovits <i>et al.</i> , 1995	1.53	Schwartz, 1986
H22	CH ₃ COOH	0.019	Davidovits <i>et al.</i> , 1995	1.24	Schwartz, 1986
H23	CH ₃ O ₂	$3.8 \cdot 10^{-3}$	$\alpha_{23} = \alpha_{16}$	1.35	Fuller, 1986 ^{a)}
H24	ETHP ^c	$8.2 \cdot 10^{-3}$	estimated	1.08	Fuller, 1986 ^{a)}
H25	Cl ₂	0.03	estimated	1.28	Schwartz, 1986
H26	Br ₂	0.03	estimated	1.00	Schwartz, 1986
H27	H ₂ SO ₄	0.07	Davidovits <i>et al.</i> , 1995	1.30	Schwartz, 1986
H28	CH ₄	$5 \cdot 10^{-5}$	estimated	1.41	Fuller, 1986 ^{a)}
H29	C ₂ H ₆	$1 \cdot 10^{-4}$	estimated	0.95	Fuller, 1986 ^{a)}
H30	C ₂ H ₄	$1 \cdot 10^{-4}$	estimated	1.01	Fuller, 1986 ^{a)}
H31	PAN ^e	0.019	$\alpha_{31} = \alpha_{22}$	0.63	Fuller, 1986 ^{a)}
H32	OP2 ^f	0.01	estimated	0.76	Fuller, 1986 ^{a)}
H33	OL2P ^g	$8.2 \cdot 10^{-3}$	$\alpha_{33} = \alpha_{24}$	0.82	Fuller, 1986 ^{a)}
H34	ACO ₃ ^h	0.019	$\alpha_{34} = \alpha_{22}$	1.0	Fuller, 1986 ^{a)}

a) These values are calculated after the method by Fuller, 1986

Table 3: HO_x- and Transition metal ion (TMI)-Chemistry

Reaction No.	Reaction	k ₂₉₈ , M ⁿ s ⁻¹	E _a / R, K	Reference
R1	H ₂ O ₂ + Fe ³⁺ → HO ₂ + H ⁺ + Fe ²⁺	2·10 ⁻³		Walling and Goosen, 1973
R2	H ₂ O ₂ + [Fe(OH)] ²⁺ → HO ₂ + H ₂ O + Fe ²⁺	2·10 ⁻³		k ₂ = k ₁
R3	H ₂ O ₂ + [Fe(OH) ₂] ⁺ → HO ₂ + OH ⁻ + Fe ²⁺ +H ₂ O	2·10 ⁻³		k ₃ = k ₁
R4	H ₂ O ₂ + Fe ²⁺ → OH + OH ⁻ + Fe ³⁺	76		Walling, 1975
R5	H ₂ O ₂ + Mn ³⁺ → HO ₂ + H ⁺ + Mn ²⁺	7.3 · 10 ⁴		Davies <i>et al.</i> , 1968
R6	H ₂ O ₂ + Cu ⁺ → OH + OH ⁻ + Cu ²⁺	7.0 · 10 ³		Berdnikov, 1973
R7	O ₂ ⁻ + Fe ³⁺ → O ₂ + Fe ²⁺	1.5 · 10 ⁸		Rush and Bielski, 1985
R8	HO ₂ + [Fe(OH)] ²⁺ → Fe ²⁺ + O ₂ + H ₂ O	1.3 · 10 ⁵		Ziajka <i>et al.</i> , 1994
R9	O ₂ ⁻ + [Fe(OH)] ²⁺ → O ₂ + Fe ²⁺ + OH ⁻	1.5 · 10 ⁸		Rush and Bielski, 1985
R10	O ₂ ⁻ + [Fe(OH) ₂] ⁺ → O ₂ + Fe ²⁺ + 2 OH ⁻	1.5 · 10 ⁸		Rush and Bielski, 1985
R11	O ₂ ⁻ + Fe ²⁺ (+ 2 H ⁺) → H ₂ O ₂ + Fe ³⁺	1.0 · 10 ⁷		Rush and Bielski, 1985
R12	HO ₂ + Fe ²⁺ (+ H ⁺) → H ₂ O ₂ + Fe ³⁺	1.2 · 10 ⁶	5050	Jayson <i>et al.</i> , 1973b
R13	OH + Fe ²⁺ → [Fe(OH)] ²⁺	4.3 · 10 ⁸	1100	Christensen and Sehested, 1981
R14	O ₂ ⁻ + Mn ²⁺ (+ H ⁺) → H ₂ O ₂ + Mn ³⁺	1.1 · 10 ⁸		Pick-Kaplan and Rabani, 1976
R15	HO ₂ + Mn ²⁺ (+ H ⁺) → H ₂ O ₂ + Mn ³⁺	2 · 10 ⁵		Graedel <i>et al.</i> , 1986
R16	OH + Mn ²⁺ → OH ⁻ + Mn ³⁺	2.6 · 10 ⁷		Baral <i>et al.</i> , 1986
R17	O ₂ ⁻ + Cu ⁺ (+ 2 H ⁺) → H ₂ O ₂ + Cu ²⁺	9.4 · 10 ⁹		von Piechowski <i>et al.</i> , 1993
R18	HO ₂ + Cu ⁺ (+ H ⁺) → H ₂ O ₂ + Cu ²⁺	2.2 · 10 ⁹		Kozlov and Berdnikov, 1973
R19	OH + Cu ⁺ → OH ⁻ + Cu ²⁺	3 · 10 ⁹		Goldstein <i>et al.</i> , 1992
R20	HO ₂ + Cu ²⁺ → O ₂ + Cu ⁺ + H ⁺	1.2 · 10 ⁹		Cabelli <i>et al.</i> , 1987
R21	O ₂ ⁻ + Cu ²⁺ → O ₂ + Cu ⁺	1.1 · 10 ¹⁰		Cabelli <i>et al.</i> , 1987
R22	Fe ³⁺ + Cu ⁺ → Fe ²⁺ + Cu ²⁺	3 · 10 ⁷		Sedlak and Hoigné, 1993
R23	[Fe(OH)] ²⁺ + Cu ⁺ → Fe ²⁺ + Cu ²⁺ + OH ⁻	3 · 10 ⁷		Sedlak and Hoigné, 1993
R24	[Fe(OH) ₂] ⁺ + Cu ⁺ → Fe ²⁺ + Cu ²⁺ + 2 OH ⁻	3 · 10 ⁷		Sedlak and Hoigné, 1993
R25	Fe ²⁺ + Mn ³⁺ → Fe ³⁺ + Mn ²⁺	1.5 · 10 ⁴		Diebler and Sutin, 1964
R26	O ₃ + O ₂ ⁻ (+ H ⁺) → 2 O ₂ + OH	1.5 · 10 ⁹		Sehested <i>et al.</i> , 1983

R27	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2$	$8.3 \cdot 10^5$	2720	Bielski <i>et al.</i> , 1985
R28	$\text{HO}_2 + \text{O}_2^- (+ \text{H}^+) \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$9.7 \cdot 10^7$	1060	Bielski <i>et al.</i> , 1985
R29	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	$1.0 \cdot 10^{10}$		Elliot and Buxton, 1992
R30	$\text{O}_2^- + \text{OH} \rightarrow \text{OH}^- + \text{O}_2$	$1.1 \cdot 10^{10}$	2120	Christensen <i>et al.</i> , 1989
R31	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{H}_2\text{O}$	$3.0 \cdot 10^7$	1680	Christensen <i>et al.</i> , 1982
R32	$\text{MHP} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$3.0 \cdot 10^{7\text{b}}$	1680 ^b	$k_{\text{R32}} = k_{\text{R31}}$
R33	$\text{HSO}_3^- + \text{OH} \rightarrow \text{H}_2\text{O} + \text{SO}_3^-$	$2.7 \cdot 10^9$		Buxton <i>et al.</i> , 1996a
R34	$\text{SO}_3^{2-} + \text{OH} \rightarrow \text{OH}^- + \text{SO}_3^-$	$4.6 \cdot 10^9$		Buxton <i>et al.</i> , 1996a

Table 4: Nitrogen-Chemistry

Reaction No.	Reaction	$k_{298},$ $M^{-n} s^{-1}$	$E_a / R,$ K	Reference
R35	$N_2O_5 + H_2O \rightarrow 2 H^+ + 2 NO_3^-$	$5 \cdot 10^9$		estimated
R36	$NO_3 + OH^- \rightarrow NO_3^- + OH$	$9.4 \cdot 10^7$	2700	Exner <i>et al.</i> , 1992
R37	$NO_3 + Fe^{2+} \rightarrow NO_3^- + Fe^{3+}$	$8 \cdot 10^6$		Pikaev <i>et al.</i> , 1974
R38	$NO_3 + Mn^{2+} \rightarrow NO_3^- + Mn^{3+}$	$1.1 \cdot 10^6$		Neta and Huie, 1986
R39	$NO_3 + H_2O_2 \rightarrow NO_3^- + H^+ + HO_2$	$4.9 \cdot 10^6$	2000	Herrmann <i>et al.</i> , 1994
R40	$NO_3 + MHP \rightarrow NO_3^- + H^+ + CH_3O_2$	$4.9 \cdot 10^6$ ^b	2000 ^b	$k_{R40} = k_{R39}$
R41	$NO_3 + HO_2 \rightarrow NO_3^- + H^+ + O_2$	$3.0 \cdot 10^9$		Sehested <i>et al.</i> , 1994
R42	$NO_3 + O_2^- \rightarrow NO_3^- + O_2$	$3 \cdot 10^9$ ^b		$k_{R42} = k_{R41}$
R43	$NO_3 + HSO_3^- \rightarrow NO_3^- + H^+ + SO_3^-$	$1.3 \cdot 10^9$	2000	Exner <i>et al.</i> , 1992
R44	$NO_3 + SO_3^{2-} \rightarrow NO_3^- + SO_3^-$	$3.0 \cdot 10^8$		Exner <i>et al.</i> , 1992
R45	$NO_3 + HSO_4^- \rightarrow NO_3^- + H^+ + SO_4^-$	$2.6 \cdot 10^5$		Raabe, 1996
R46	$NO_3 + SO_4^{2-} \rightarrow NO_3^- + SO_4^-$	$5.6 \cdot 10^3$		Logager <i>et al.</i> , 1993
R47	$NO_2 + OH \rightarrow NO_3^- + H^+$	$1.2 \cdot 10^{10}$		Wagner <i>et al.</i> , 1980
R48	$NO_2 + O_2^- \rightarrow NO_2^- + O_2$	$1 \cdot 10^8$		Warneck and Wurzinger, 1988
R49	$NO_2 + NO_2 (+ H_2O) \rightarrow HNO_2 + NO_3^- + H^+$	$8.4 \cdot 10^7$	-2900	Park and Lee, 1988
R50	$O_2NO_2^- \rightarrow NO_2^- + O_2$	$4.5 \cdot 10^{-2}$		Lammel <i>et al.</i> , 1990
R51	$NO_2^- + OH \rightarrow NO_2 + OH^-$	$1.1 \cdot 10^{10}$		Barker <i>et al.</i> , 1970
R52	$NO_2^- + SO_4^- \rightarrow SO_4^{2-} + NO_2$	$7.2 \cdot 10^8$		Reese, 1997
R53	$NO_2^- + NO_3 \rightarrow NO_3^- + NO_2$	$1.4 \cdot 10^9$	0	Herrmann and Zellner, 1998
R54	$NO_2^- + Cl_2^- \rightarrow 2 Cl^- + NO_2$	$6 \cdot 10^7$		Jacobi, 1996
R55	$NO_2^- + Br_2^- \rightarrow 2 Br^- + NO_2$	$1.2 \cdot 10^7$	1720	Shoute <i>et al.</i> , 1991
R56	$NO_2^- + CO_3^- \rightarrow CO_3^{2-} + NO_2$	$6.6 \cdot 10^5$	850	Huie <i>et al.</i> , 1991a
R57	$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	$5 \cdot 10^5$	7000	Damschen and Martin, 1983
R58	$HNO_2 + OH \rightarrow NO_2 + H_2O$	$1 \cdot 10^9$		Rettich, 1978
R59	$HNO_4 + HSO_3^- \rightarrow HSO_4^- + NO_3$	$3.5 \cdot 10^5$		Amels <i>et al.</i> , 1996

Table 5: Sulfur-Chemistry

Reaction No.	Reaction	k_{298} , $M^{-n} s^{-1}$	E_a / R , K	Reference
R60	$HMS^- + OH^- (+ O_2 + H_2O) \rightarrow H_2O + HO_2 + HCOOH + HSO_3^-$	$3 \cdot 10^8$		Buxton, 1994
R61	$HMS^- + SO_4^{2-} \rightarrow SO_4^{2-} + H^+ + HCHO + SO_3^-$	$2.8 \cdot 10^6$		Buxton, 1994
R62	$HMS^- + NO_3^- \rightarrow NO_3^- + H^+ + HCHO + SO_3^-$	$4.2 \cdot 10^6$		Herrmann and Zellner, 1998
R63	$HMS^- + Cl_2^- \rightarrow 2 Cl^- + H^+ + HCHO + SO_3^-$	$5.0 \cdot 10^5$		Jacobi, 1996
R64	$HMS^- + Br_2^- \rightarrow 2 Br^- + H^+ + HCHO + SO_3^-$	$5 \cdot 10^4$		estimated
R65	$HSO_3^- + H_2O_2 + H^+ \rightarrow SO_4^{2-} + H_2O + 2 H^+$	$6.9 \cdot 10^7$	4000	Lind <i>et al.</i> , 1987
R66	$HSO_3^- + CH_3OOH + H^+ \rightarrow SO_4^{2-} + 2 H^+ + CH_3OH$	$1.8 \cdot 10^7$	3800	Lind <i>et al.</i> , 1987
R67	$HSO_3^- + CH_3C(O)OOH + H^+ \rightarrow SO_4^{2-} + 2 H^+ + P$	$4.8 \cdot 10^7$	3990	Lind <i>et al.</i> , 1987
R68	$SO_2 + O_3 (+H_2O) \rightarrow HSO_4^- + O_2 + H^+$	$2.4 \cdot 10^4$		Hoffmann, 1986
R69	$HSO_3^- + O_3 \rightarrow HSO_4^- + O_2$	$3.7 \cdot 10^5$	5530	Hoffmann, 1986
R70	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	$1.5 \cdot 10^9$	5280	Hoffmann, 1986
R71	$[Fe(OH)]^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	39		Ziajka <i>et al.</i> , 1994
R72	$Fe^{2+} + SO_5^- (+H_2O) \rightarrow [Fe(OH)]^{2+} + HSO_5^-$	$4.3 \cdot 10^7$		Herrmann <i>et al.</i> , 1996
R73	$Fe^{2+} + HSO_5^- \rightarrow [Fe(OH)]^{2+} + SO_4^-$	$3 \cdot 10^4$		Ziajka <i>et al.</i> , 1994
R74	$Mn^{2+} + SO_5^- (+H_2O) \rightarrow Mn^{3+} + HSO_5^- + OH^-$	$4.6 \cdot 10^6$		Herrmann <i>et al.</i> , 1996
R75	$Fe^{2+} + SO_4^- (+H_2O) \rightarrow [Fe(OH)]^{2+} + SO_4^{2-} + H^+$	$3.5 \cdot 10^7$		Ziajka <i>et al.</i> , 1994
R76	$Fe^{2+} + S_2O_8^{2-} (+H_2O) \rightarrow [Fe(OH)]^{2+} + SO_4^{2-} + SO_4^- + H^+$	17		Buxton <i>et al.</i> , 1997
R77	$SO_5^- + SO_5^- \rightarrow S_2O_8^{2-} + O_2$	$1.8 \cdot 10^8$	2600	Herrmann <i>et al.</i> , 1995
R78	$SO_5^- + SO_5^- \rightarrow 2 SO_4^- + O_2$	$7.2 \cdot 10^6$	2600	Herrmann <i>et al.</i> , 1995
R79	$SO_5^- + HO_2 \rightarrow HSO_5^- + O_2$	$1.7 \cdot 10^9$		Buxton <i>et al.</i> , 1996b
R80	$SO_5^- + O_2^- (+H_2O) \rightarrow HSO_5^- + OH^- + O_2$	$1.7 \cdot 10^9$		$k_{R80} = k_{R79}$
R81	$SO_3^- + O_2 \rightarrow SO_5^-$	$2.5 \cdot 10^9$		Buxton <i>et al.</i> , 1996a
R82	$SO_5^- + HSO_3^- \rightarrow HSO_5^- + SO_3^-$	$8.6 \cdot 10^3$		Buxton <i>et al.</i> , 1996a
R83	$SO_5^- + HSO_3^- \rightarrow SO_4^{2-} + SO_4^- + H^+$	$3.6 \cdot 10^2$		Buxton <i>et al.</i> , 1996a
R84	$SO_5^- + SO_3^{2-} (+H^+) \rightarrow HSO_5^- + SO_3^-$	$2.13 \cdot 10^5$		Buxton <i>et al.</i> , 1996a
R85	$SO_5^- + SO_3^{2-} \rightarrow SO_4^- + SO_4^{2-}$	$5.5 \cdot 10^5$		Buxton <i>et al.</i> , 1996a
R86	$OH + HSO_4^- \rightarrow H_2O + SO_4^-$	$3.5 \cdot 10^5$		Tang <i>et al.</i> , 1988

R87	$\text{SO}_4^- + \text{SO}_4^- \rightarrow \text{S}_2\text{O}_8^{2-}$	$1.6 \cdot 10^8$		Herrmann <i>et al.</i> , 1995a
R88	$\text{SO}_4^- + \text{HSO}_3^- \rightarrow \text{SO}_4^{2-} + \text{SO}_3^- + \text{H}^+$	$3.2 \cdot 10^8$		Reese, 1997
R89	$\text{SO}_4^- + \text{SO}_3^{2-} \rightarrow \text{SO}_4^{2-} + \text{SO}_3^-$	$3.2 \cdot 10^8$	1200	Reese, 1997
R90	$\text{SO}_4^- + \text{Fe}^{2+} \rightarrow [\text{Fe}(\text{SO}_4)]^+$	$3 \cdot 10^8$		McElroy and Waygood, 1990
R91	$\text{SO}_4^- + \text{Mn}^{2+} \rightarrow \text{SO}_4^{2-} + \text{Mn}^{3+}$	$2 \cdot 10^7$		Neta and Huie, 1986
R92	$\text{SO}_4^- + \text{Cu}^+ \rightarrow \text{SO}_4^{2-} + \text{Cu}^{2+}$	$3 \cdot 10^8$ ^b		$k_{R92} = k_{R90}$
R93	$\text{SO}_4^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2$	$2.8 \cdot 10^7$		Reese, 1997
R94	$\text{SO}_4^- + \text{MHP} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{O}_2$	$2.8 \cdot 10^7$ ^b		$k_{R94} = k_{R93}$
R95	$\text{SO}_4^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{O}_2$	$3.5 \cdot 10^9$		Jiang <i>et al.</i> , 1992
R96	$\text{SO}_4^- + \text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{O}_2$	$3.5 \cdot 10^9$ ^b		$k_{R96} = k_{R95}$
R97	$\text{SO}_4^- + \text{NO}_3^- \rightarrow \text{SO}_4^{2-} + \text{NO}_3$	$5.0 \cdot 10^4$		Exner <i>et al.</i> , 1992
R98	$\text{SO}_4^- + \text{OH}^- \rightarrow \text{SO}_4^{2-} + \text{OH}$	$1.4 \cdot 10^7$		Herrmann <i>et al.</i> , 1995
R99	$\text{SO}_4^- + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}$	11	1110	Herrmann <i>et al.</i> , 1995
R100	$\text{HSO}_5^- + \text{HSO}_3^- + \text{H}^+ \rightarrow 2 \text{SO}_4^{2-} + 3 \text{H}^+$	$7.14 \cdot 10^6$		Betterton and Hoffmann, 1988b
R101	$\text{HSO}_5^- + \text{SO}_3^{2-} + \text{H}^+ \rightarrow 2 \text{SO}_4^{2-} + 2 \text{H}^+$	$7.14 \cdot 10^6$		Betterton and Hoffmann, 1988b
R102	$\text{HSO}_5^- + \text{OH}^- \rightarrow \text{SO}_5^- + \text{H}_2\text{O}$	$1.7 \cdot 10^7$		Maruthamuthu and Neta, 1977

Table 6: Organic Chemistry

Reaction No.	Reaction	k_{298} , $M^{-n} s^{-1}$	E_a / R , K	Reference
R103	$CH_3OH + OH (+ O_2) \rightarrow H_2O + HO_2 + HCHO$	$1.0 \cdot 10^9$	580	Elliot and McCracken, 1989
R104	$CH_3OH + SO_4^- (+ O_2) \rightarrow SO_4^{2-} + H^+ + HO_2 + HCHO$	$9.0 \cdot 10^6$	2190	Clifton and Huie, 1989
R105	$CH_3OH + NO_3 (+ O_2) \rightarrow NO_3^- + H^+ + HO_2 + HCHO$	$5.4 \cdot 10^5$	4300	Herrmann and Zellner, 1998
R106	$CH_3OH + Cl_2^- (+ O_2) \rightarrow 2 Cl^- + H^+ + HO_2 + HCHO$	1000	5500	Zellner <i>et al.</i> , 1996
R107	$CH_3OH + Br_2^- (+ O_2) \rightarrow 2 Br^- + H^+ + HO_2 + HCHO$	$5.4 \cdot 10^5$		Wicktor, 1997
R108	$CH_3OH + CO_3^- (+ O_2) \rightarrow CO_3^{2-} + H^+ + HO_2 + HCHO$	$2.6 \cdot 10^3$		Zellner <i>et al.</i> , 1996
R109	$ETOH + OH (+ O_2) \rightarrow H_2O + HO_2 + CH_3CHO$	$1.9 \cdot 10^9$		Buxton <i>et al.</i> , 1988a
R110	$ETOH + SO_4^- (+ O_2) \rightarrow SO_4^{2-} + H^+ + HO_2 + CH_3CHO$	$4.1 \cdot 10^7$	1760	Clifton and Huie, 1989
R111	$ETOH + NO_3 (+ O_2) \rightarrow NO_3^- + H^+ + HO_2 + CH_3CHO$	$2.2 \cdot 10^6$	3300	Herrmann and Zellner, 1998
R112	$ETOH + Cl_2^- (+ O_2) \rightarrow 2 Cl^- + H^+ + HO_2 + CH_3CHO$	$1.2 \cdot 10^5$		Zellner <i>et al.</i> , 1996
R113	$ETOH + Br_2^- (+ O_2) \rightarrow 2 Br^- + H^+ + HO_2 + CH_3CHO$	$3.8 \cdot 10^3$		Reese <i>et al.</i> , 1999
R114	$ETOH + CO_3^- (+ O_2) \rightarrow CO_3^{2-} + H^+ + HO_2 + CH_3CHO$	$1.5 \cdot 10^4$		Khuz'min, 1972
R115	$CH_2(OH)_2 + OH (+ O_2) \rightarrow H_2O + HO_2 + HCOOH$	$1.0 \cdot 10^9$	1020	Hart <i>et al.</i> , 1964; Chin and Wine, 1994
R116	$CH_2(OH)_2 + SO_4^- (+ O_2) \rightarrow SO_4^{2-} + H^+ + HO_2 + HCOOH$	$1.4 \cdot 10^7$	1300	Buxton <i>et al.</i> , 1990
R117	$CH_2(OH)_2 + NO_3 (+ O_2) \rightarrow NO_3^- + H^+ + HO_2 + HCOOH$	$1.0 \cdot 10^6$	4500	Exner <i>et al.</i> , 1993
R118	$CH_2(OH)_2 + Cl_2^- (+ O_2) \rightarrow 2 Cl^- + H^+ + HO_2 + HCOOH$	$3.1 \cdot 10^4$	4400	Zellner <i>et al.</i> , 1996
R119	$CH_2(OH)_2 + Br_2^- (+ O_2) \rightarrow 2 Br^- + H^+ + HO_2 + HCOOH$	$3 \cdot 10^3$ ^b		estimated
R120	$CH_2(OH)_2 + CO_3^- (+ O_2) \rightarrow CO_3^{2-} + H^+ + HO_2 + HCOOH$	$1.3 \cdot 10^4$		Zellner <i>et al.</i> , 1996
R121	$CH_3CH(OH)_2 + OH (+ O_2) \rightarrow H_2O + HO_2 + HAc$	$1.2 \cdot 10^9$		Schuchmann and von Sonntag, 1988
R122	$CH_3CHO + OH (+ O_2 + H_2O) \rightarrow H_2O + HO_2 + HAc$	$3.6 \cdot 10^9$		Schuchmann and von Sonntag, 1988
R123	$CH_3CH(OH)_2 + SO_4^- (+ O_2) \rightarrow SO_4^{2-} + H^+ + HO_2 + HAc$	$2 \cdot 10^7$ ^b		estimated
R124	$CH_3CH(OH)_2 + NO_3 (+ O_2) \rightarrow NO_3^- + H^+ + HO_2 + HAc$	$1.9 \cdot 10^6$		Zellner <i>et al.</i> , 1996
R125	$CH_3CH(OH)_2 + Cl_2^- (+ O_2) \rightarrow 2 Cl^- + H^+ + HO_2 + HAc$	$4 \cdot 10^4$		Jacobi, 1996
R126	$CH_3CH(OH)_2 + Br_2^- (+ O_2) \rightarrow 2 Br^- + H^+ + HO_2 + HAc$	$4 \cdot 10^4$		estimated
R127	$CH_3CH(OH)_2 + CO_3^- (+ O_2) \rightarrow CO_3^{2-} + H^+ + HO_2 + HAc$	$1 \cdot 10^4$		estimated
R128	$HCOOH + OH (+ O_2) \rightarrow H_2O + HO_2 + CO_2$	$1.3 \cdot 10^8$	1000	Buxton <i>et al.</i> , 1988a; Chin and Wine, 1994
R129	$HCOO^- + OH (+ O_2) \rightarrow OH^- + HO_2 + CO_2$	$4 \cdot 10^9$	1000	Buxton <i>et al.</i> , 1988a;

R130	$\text{HCOOH} + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 + \text{CO}_2$	$2.5 \cdot 10^6$		Elliot and Simsons, 1984
R131	$\text{HCOO}^- + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{HO}_2 + \text{CO}_2$	$2.1 \cdot 10^7$		Reese, 1997
R132	$\text{HCOOH} + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$	$3.8 \cdot 10^5$	3400	Reese, 1997
R133	$\text{HCOO}^- + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{HO}_2 + \text{CO}_2$	$5.1 \cdot 10^7$	2200	Exner <i>et al.</i> , 1994
R134	$\text{HCOOH} + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$	5500	4500	Exner <i>et al.</i> , 1994
R135	$\text{HCOO}^- + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{HO}_2 + \text{CO}_2$	$1.3 \cdot 10^6$		Jacobi <i>et al.</i> , 1999
R136	$\text{HCOOH} + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$	$4 \cdot 10^3$		Jacobi <i>et al.</i> , 1996
R137	$\text{HCOO}^- + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{HO}_2 + \text{CO}_2$	$4.9 \cdot 10^3$		Reese <i>et al.</i> , 1999
R138	$\text{HCOO}^- + \text{CO}_3^- (+ \text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{HO}_2 + \text{CO}_2$	$1.4 \cdot 10^5$	3300	Jacobi, 1996
R139	$\text{HAc} + \text{OH} (+ \text{O}_2) \rightarrow \text{H}_2\text{O} + \text{ACO}_3 + \text{CO}_2$	$1.5 \cdot 10^7$	1330	Zellner <i>et al.</i> , 1996
R140	$\text{Ac}^- + \text{OH} (+ \text{O}_2) \rightarrow \text{OH}^- + \text{ACO}_3 + \text{CO}_2$	$1.0 \cdot 10^9$	1800	Thomas, 1965; Chin and Wine, 1994
R141	$\text{HAc} + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{ACO}_3 + \text{CO}_2$	$2.0 \cdot 10^5$		Fisher and Hamill, 1973; Chin and Wine, 1994
R142	$\text{Ac}^- + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$	$2.8 \cdot 10^7$	1210	Reese, 1997
R143	$\text{HAc} + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{H}^+ + \text{ACO}_3 + \text{CO}_2$	$1.4 \cdot 10^4$	3800	Reese, 1997; Huie and Clifton, 1990
R144	$\text{Ac}^- + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{CH}_3\text{O}_2 + \text{CO}_2$	$2.9 \cdot 10^6$	3800	Exner <i>et al.</i> , 1994
R145	$\text{HAc} + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{ACO}_3 + \text{CO}_2$	1950	4800	Exner <i>et al.</i> , 1994
R146	$\text{Ac}^- + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{CH}_3\text{O}_2 + \text{CO}_2$	$2.6 \cdot 10^5$	4800	Jacobi <i>et al.</i> , 1998
R147	$\text{HAc} + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{ACO}_3 + \text{CO}_2$	10		Jacobi <i>et al.</i> , 1996
R148	$\text{Ac}^- + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{CH}_3\text{O}_2 + \text{CO}_2$	100		Reese <i>et al.</i> , 1999
R149	$\text{Ac}^- + \text{CO}_3^- (+ \text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$	580		Jacobi, 1996
R150	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{O}_2$	$1.7 \cdot 10^8$	2200	Zellner <i>et al.</i> , 1996
R151	$\text{CH}_3\text{O}_2 + \text{HSO}_3^- \rightarrow \text{MHP} + \text{SO}_3^-$	$5 \cdot 10^5$		Herrmann <i>et al.</i> , 1999b)
R152	$\text{ETHP} + \text{ETHP} \rightarrow \text{Prod.}$	$1.5 \cdot 10^8$ c	-1500	Herrmann <i>et al.</i> , 1999b)

Table 7: Chlorine chemistry

Reaction No.	Reaction	k_{298} , $M^{-n} s^{-1}$	E_a / R , K	Reference
R153	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	$3.3 \cdot 10^8$	0	Huie and Clifton, 1990; Herrmann <i>et al.</i> , 1997
R154	$NO_3 + Cl^- \rightarrow NO_3^- + Cl$	$1.0 \cdot 10^7$	4300	Exner <i>et al.</i> , 1992
R155	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2 Cl^-$	$8.7 \cdot 10^8$		Zellner <i>et al.</i> , 1996
R156	$Cl_2^- + Fe^{2+} \rightarrow 2 Cl^- + Fe^{3+}$	$1.0 \cdot 10^7$	3030	Thornton and Laurence, 1973
R157	$Cl_2^- + Mn^{2+} \rightarrow 2 Cl^- + Mn^{3+}$	$8.5 \cdot 10^6$	4090	Laurence and Thornton, 1973
R158	$Cl_2^- + Cu^+ \rightarrow 2 Cl^- + Cu^{2+}$	$1 \cdot 10^7$		$k_{R158} = k_{R156}$
R159	$Cl_2^- + H_2O_2 \rightarrow 2 Cl^- + H^+ + HO_2$	$7.0 \cdot 10^5$	3340	Elliot, 1989
R160	$Cl_2^- + MHP \rightarrow 2 Cl^- + H^+ + CH_3O_2$	$7.0 \cdot 10^5$	3340	$k_{R160} = k_{R159}$
R161	$Cl_2^- + OH^- \rightarrow 2 Cl^- + OH$	$4.0 \cdot 10^6$		Jacobi, 1996
R162	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+ + O_2$	$1.3 \cdot 10^{10}$		Jacobi, 1996
R163	$Cl_2^- + O_2^- \rightarrow 2 Cl^- + O_2$	$6 \cdot 10^9$		Jacobi, 1996
R164	$Cl_2^- + HSO_3^- \rightarrow 2 Cl^- + H^+ + SO_3^-$	$1.7 \cdot 10^8$	400	Jacobi <i>et al.</i> , 1996
R165	$Cl_2^- + SO_3^{2-} \rightarrow 2 Cl^- + SO_3^-$	$6.2 \cdot 10^7$		Jacobi <i>et al.</i> , 1996
R166	$Cl_2 + H_2O \rightarrow H^+ + Cl^- + HOCl$	0.401	7900	Wang and Margerum, 1994

Table 8: Bromine chemistry

Reaction No.	Reaction	k_{298} , $M^{-n} s^{-1}$	E_a / R , K	Reference
R167	$SO_4^- + Br^- \rightarrow SO_4^{2-} + Br$	$2.1 \cdot 10^9$		Herrmann <i>et al.</i> , 1997
R168	$NO_3 + Br^- \rightarrow NO_3^- + Br$	$3.8 \cdot 10^9$		Zellner <i>et al.</i> , 1996
R169	$Br_2^- + Br_2^- \rightarrow Br_2 + 2 Br^-$	$1.7 \cdot 10^9$		Reese, 1998
R170	$Br_2^- + Fe^{2+} \rightarrow 2 Br^- + Fe^{3+}$	$3.6 \cdot 10^6$	3330	Thornton and Laurence, 1973
R171	$Br_2^- + Mn^{2+} \rightarrow 2 Br^- + Mn^{3+}$	$6.3 \cdot 10^6$	4330	Laurence and Thornton, 1973
R172	$Br_2^- + Cu^+ \rightarrow 2 Br^- + Cu^{2+}$	$3.6 \cdot 10^6$		$k_{R172} = k_{R170}$
R173	$Br_2^- + H_2O_2 \rightarrow 2 Br^- + H^+ + HO_2$	$1.0 \cdot 10^5$		Reese, 1997
R174	$Br_2^- + MHP \rightarrow 2 Br^- + H^+ + CH_3O_2$	$1.0 \cdot 10^5$		$k_{R174} = k_{R172}$
R175	$Br_2^- + OH^- \rightarrow 2 Br^- + OH$	$1.1 \cdot 10^4$		Jacobi, 1996
R176	$Br_2^- + HO_2 \rightarrow 2 Br^- + H^+ + O_2$	$6.5 \cdot 10^9$		Rafi and Sutton, 1965
R177	$Br_2^- + O_2^- \rightarrow 2 Br^- + O_2$	$1.7 \cdot 10^8$		Wagner and Strehlow, 1987
R178	$Br_2^- + HSO_3^- \rightarrow 2 Br^- + H^+ + SO_3^-$	$5.0 \cdot 10^7$	780	Shoute <i>et al.</i> , 1991
R179	$Br_2^- + SO_3^{2-} \rightarrow 2 Br^- + SO_3^-$	$3.3 \cdot 10^7$	650	Shoute <i>et al.</i> , 1991
R180	$Br_2 + H_2O \rightarrow Br^- + H^+ + HOBr$	1.7	7500	Beckwith <i>et al.</i> , 1996

Table 9: Carbonate chemistry

Reaction No.	Reaction ^a	$k_{298},$ $M^{-n} s^{-1}$	$E_a / R,$ K	Reference
R181	$HCO_3^- + OH^- \rightarrow H_2O + CO_3^{2-}$	$1.7 \cdot 10^7$	1900	Exner, 1990
R182	$CO_3^{2-} + OH^- \rightarrow OH^- + CO_3^{2-}$	$3.9 \cdot 10^8$	2840	Buxton <i>et al.</i> , 1988a,b
R183	$CO_3^{2-} + SO_4^{2-} \rightarrow SO_4^{2-} + CO_3^{2-}$	$4.1 \cdot 10^7$		estimated
R184	$HCO_3^- + SO_4^{2-} \rightarrow SO_4^{2-} + CO_3^{2-} + H^+$	$2.8 \cdot 10^6$	2090	Huie and Clifton, 1990
R185	$CO_3^{2-} + NO_3^- \rightarrow NO_3^- + CO_3^{2-}$	$4.1 \cdot 10^7$		estimated
R186	$CO_3^{2-} + Cl_2^- \rightarrow 2 Cl^- + CO_3^{2-}$	$2.7 \cdot 10^6$		estimated
R187	$CO_3^{2-} + Br_2^- \rightarrow 2 Br^- + CO_3^{2-}$	$1.1 \cdot 10^5$		Huie <i>et al.</i> , 1991b
R188	$CO_3^- + CO_3^- (+O_2) \rightarrow 2 O_2^- + 2 CO_2$	$2.2 \cdot 10^6$		Huie and Clifton, 1990
R189	$CO_3^- + Fe^{2+} \rightarrow CO_3^{2-} + Fe^{3+}$	$2 \cdot 10^7$		estimated
R190	$CO_3^- + Mn^{2+} \rightarrow CO_3^{2-} + Mn^{3+}$	$1.5 \cdot 10^7$		Cope <i>et al.</i> , 1978
R191	$CO_3^- + Cu^+ \rightarrow CO_3^{2-} + Cu^{2+}$	$2 \cdot 10^7$		estimated
R192	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	$4.3 \cdot 10^5$		Draganic <i>et al.</i> , 1991
R193	$CO_3^- + MHP \rightarrow HCO_3^- + CH_3O_2$	$4.3 \cdot 10^5$		$k_{R193} = k_{R192}$
R194	$CO_3^- + HO_2 \rightarrow HCO_3^- + O_2$	$6.5 \cdot 10^8$		$k_{R194} = k_{R195}$
R195	$CO_3^- + O_2^- \rightarrow CO_3^{2-} + O_2$	$6.5 \cdot 10^8$		Eriksen <i>et al.</i> , 1985
R196	$CO_3^- + HSO_3^- \rightarrow HCO_3^- + SO_3^-$	$1 \cdot 10^7$		estimated
R197	$CO_3^- + SO_3^{2-} \rightarrow CO_3^{2-} + SO_3^-$	$5.0 \cdot 10^6$	470	Huie <i>et al.</i> , 1991a

Table 10: CAPRAM: Aqueous phase equilibria

No.	Reaction	K M ^Z	k(forward) M ⁻ⁿ s ⁻¹	E _a / R, K		k(back) M ⁻ⁿ s ⁻¹	E _a / R, K	
E1	H ₂ O ⇌ H ⁺ + OH ⁻	1.8·10 ⁻¹⁴	2.34 · 10 ⁻⁵	6800	a	1.3 · 10 ¹¹		c
E2	CO ₂ + H ₂ O ⇌ H ₂ CO ₃	7.7·10 ⁻⁷	4.3·10 ⁻²	9250	b	5.6·10 ⁴	8500	x
E3	H ₂ CO ₃ ⇌ H ⁺ + HCO ₃ ⁻	2·10 ⁻⁴	1 · 10 ⁷		c	5 · 10 ¹⁰		c
E4	HCO ₃ ⁻ ⇌ H ⁺ + CO ₃ ²⁻	4.69·10 ⁻¹¹	2.35	1820	a	5 · 10 ¹⁰		c
E5	HCl ⇌ H ⁺ + Cl ⁻	1.72·10 ⁶	8.6 · 10 ¹⁶	-6890	d	5 · 10 ¹⁰		c
E6	NH ₃ + H ₂ O ⇌ NH ₄ ⁺ + OH ⁻	1.77·10 ⁻⁵	6.02 · 10 ⁵	560	a	3.4 · 10 ¹⁰		c
E7	HO ₂ ⇌ H ⁺ + O ₂ ⁻	1.6·10 ⁻⁵	8.0 · 10 ⁵	0	e f	5 · 10 ¹⁰	0	y
E8	HNO ₃ ⇌ H ⁺ + NO ₃ ⁻	22	1.1 · 10 ¹²	-1800	g h	5 · 10 ¹⁰		c
E9	HNO ₂ ⇌ H ⁺ + NO ₂ ⁻	5.3·10 ⁻⁴	2.65 · 10 ⁷	1760	i	5 · 10 ¹⁰		c
E10	HO ₂ NO ₂ ⇌ H ⁺ + O ₂ NO ₂ ⁻	1·10 ⁻⁵	5 · 10 ⁵		j	5 · 10 ¹⁰		y
E11	NO ₂ + HO ₂ ⇌ HO ₂ NO ₂	2.2·10 ⁹	1.0 · 10 ⁷		k	4.6 · 10 ⁻³		k
E12	SO ₂ + H ₂ O ⇌ HSO ₃ ⁻ + H ⁺	3.13·10 ⁻⁴	6.27 · 10 ⁴	-1940	l	2.0 · 10 ⁸		c
E13	HSO ₃ ⁻ ⇌ SO ₃ ²⁻ + H ⁺	6.22·10 ⁻⁸	3110	-1960	l	5 · 10 ¹⁰		c
E14	HSO ₄ ⁻ ⇌ SO ₄ ²⁻ + H ⁺	1.02·10 ⁻²	1.02 · 10 ⁹	-2700	g	1 · 10 ¹¹		c
E15	HCOOH ⇌ HCOO ⁻ + H ⁺	1.77·10 ⁻⁴	8.85 · 10 ⁶	-12	a	5 · 10 ¹⁰		c
E16	HAc ⇌ Ac ⁻ + H ⁺	1.75·10 ⁻⁵	8.75 · 10 ⁵	-46	a	5 · 10 ¹⁰		c
E17	Fe ³⁺ + H ₂ O ⇌ [Fe(OH)] ²⁺ + H ⁺	1.1·10 ⁻⁴	4.7 · 10 ⁴		m	4.3 · 10 ⁸		m
E18	[Fe(OH)] ²⁺ + H ₂ O ⇌ [Fe(OH) ₂] ⁺ + H ⁺	1.4·10 ⁻⁷	1.1 · 10 ³		n	8.0 · 10 ⁹		n
E19	Fe ³⁺ + SO ₄ ²⁻ ⇌ [Fe(SO ₄)] ⁺	1.8·10 ⁻²	3.2 · 10 ³		m	1.8 · 10 ⁵		m
E20	HCHO + H ₂ O ⇌ CH ₂ (OH) ₂	36	0.18	-4030	o	5.1 · 10 ⁻³		o
E21	CH ₃ CHO + H ₂ O ⇌ CH ₃ CH(OH) ₂	2.46·10 ⁻²	1.4 · 10 ⁻⁴	-2500	p	5.69 · 10 ⁻³		p
E22	CH ₂ (OH) ₂ + HSO ₃ ⁻ ⇌ HMS ⁻ + H ₂ O	2·10 ⁸	790	2990	q	3.95·10 ⁻⁶	2990	q
E23	CH ₂ (OH) ₂ + SO ₃ ²⁻ ⇌ HMS ⁻ + OH ⁻	3.6·10 ⁶	2.5 · 10 ⁷	2450	r	3.95 · 10 ⁻⁶	5530	q
E24	Cl + Cl ⁻ ⇌ Cl ₂ ⁻	1.9·10 ⁵	2.7 · 10 ¹⁰		r	1.4 · 10 ⁵		t
E25	Br + Br ⁻ ⇌ Br ₂ ⁻	6·10 ⁵	1.2 · 10 ¹⁰		s	1.9 · 10 ⁴		s

E26	$\text{Cl}^- + \text{OH}^- \rightleftharpoons \text{ClOH}^-$	0.7	$4.3 \cdot 10^9$	t	$6.1 \cdot 10^9$	t
E27	$\text{ClOH}^- + \text{H}^+ \rightleftharpoons \text{Cl} + \text{H}_2\text{O}$	$1.6 \cdot 10^7$	$2.1 \cdot 10^{10}$	t	$1.3 \cdot 10^3$	t
E28	$\text{ClOH}^- + \text{Cl}^- \rightleftharpoons \text{Cl}_2^- + \text{OH}^-$	$2.2 \cdot 10^{-4}$	$1.0 \cdot 10^4$	u	$4.5 \cdot 10^7$	u
E29	$\text{Br}^- + \text{OH}^- \rightleftharpoons \text{BrOH}^-$	333	$1.1 \cdot 10^{10}$	v	$3.3 \cdot 10^7$	v
E30	$\text{BrOH}^- + \text{H}^+ \rightleftharpoons \text{Br} + \text{H}_2\text{O}$	$1.8 \cdot 10^{12}$	$4.4 \cdot 10^{10}$	w	$2.45 \cdot 10^{-2}$	w
E31	$\text{BrOH}^- + \text{Br}^- \rightleftharpoons \text{Br}_2^- + \text{OH}^-$	70	$1.9 \cdot 10^8$	w	$2.7 \cdot 10^6$	w

^a Harned and Owen, 1958; ^b Welch *et al.*, 1969; ^c Graedel and Weschler, 1981; ^d Marsh and McElroy, 1985; ^e Bielski *et al.*, 1985; ^f Baxendale *et al.*, 1971; ^g Redlich, 1946; ^h Redlich and Hood, 1957; ⁱ Park and Lee, 1988; ^j Lammel *et al.*, 1990; ^k Warneck and Wurzinger, 1988; ^l Beilke and Gravenhorst, 1978; ^m Brandt and van Eldik, 1995; ⁿ Hemmes *et al.*, 1971; ^o Bell and Evans, 1966; ^p Bell *et al.*, 1956; ^q Olson and Hoffmann, 1989; ^r Jacobi *et al.*, 1997; ^s Merényi and Lind, 1994; ^t Jayson *et al.*, 1973; ^u Grigor'ev *et al.*, 1987; ^v Klaning and Wolff, 1985; ^w Fournier de Violet, 1981; ^x Sirs, 1958; ^y estimated ;

Table 11: Photolysis Rates (Aqueous Phase), geographical latitude of 51° N.

Reaction No.	Reaction	J [s ⁻¹]	Range of Quantum Yield Φ	References
P1	H ₂ O ₂ + hv → 2 OH	7.19 · 10 ⁻⁶	0.98 ± 0.03 ^a 0.96 ± 0.03 ^b	Zellner et al., 1990 Zellner et al., 1990
P2	[Fe(OH)] ²⁺ + hv → Fe ²⁺ + OH	4.51 · 10 ⁻³	0.312 ± 0.03 ... 0.074 ± 0.015 ^c	Benkelberg and Warneck, 1995
P3	[Fe(OH) ₂] ⁺ + hv → Fe ²⁺ + OH + OH ⁻	5.77 · 10 ⁻³	0.255...0.07 ^d	Benkelberg et al., 1991
P4	[Fe(SO ₄)] ⁺ + hv → Fe ²⁺ + SO ₄ ⁻	6.43 · 10 ⁻³	(7.9 ± 0.34...1.56 ± 0.02) · 10 ⁻³ ^c	Benkelberg and Warneck, 1995
P5	NO ₂ ⁻ + hv (+H ⁺) → NO + OH	2.57 · 10 ⁻⁵	0.07 ± 0.01 ^a 0.046 ± 0.009 ^b	Zellner et al., 1990 Zellner et al., 1990
P6	NO ₃ ⁻ + hv (+H ⁺) → NO ₂ + OH	4.28 · 10 ⁻⁷	0.017 ± 0.003	Zellner et al., 1990

^a λ = 308 nm, T = 298 K; ^b λ = 351 nm, T = 298 K; ^c λ = 280 ... 370 nm; ^d λ = 290...365 nm

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