CAPRAM2.3 ⇔ CAPRAM2.4(MODAC-mechanism) ⇔ CAPRAM2.4 (MODAC-mechanism) -reduced

xxx in version CAPRAM2.3, removed in CAPRAM2.4 (MODAC-mechanism)
xxx added in CAPRAM2.4 (MODAC-mechanism)
* removed in CAPRAM2.4 (MODAC-mechanism)-reduced

Table 1: Initial Concentrations for three scenarios under polluted continental (urban), unpolluted continental (remote) and marine conditions

	urban			remote			marine		
Gas phase species [ppb]									
	1st data set	2nd data set*)		1st data set	2nd data set*)		1st data set	2nd data set*)	
NO_2	4.5		a	1.5		a	0.4	0.1	a
HNO_3	1		b	0.3		b	0.15		g
CH_4	1700		a	1700		a	1700		a
H_2O_2	1		d	0.001	1	a	0.001	1	a
H_2	2000	500		2000	500		2000	500	
CO	200	300		150			140		
O_3	90		a	60	40	a	40	30	a
HCl	6	0.2	a	0.7	0.1	b	0.5		g
NH_3	25	5	a	1.5		b	0.05		g
CO_2	$5 \cdot 10^5$	$3.57 \cdot 10^5$	a	$3.3 \cdot 10^5$	$3.57 \cdot 10^5$	b	$3.3 \cdot 10^5$	$3.57 \cdot 10^5$	b
SO_2	10	5	h	1		h	0.1		h
HCHO	0.1	1	a	0.1	0.5	a	0.01	0.5	a
C_2H_6	2		a	1.5		a	1	0.5	a
HC3: Alkanes with OH rate constant between $2.7 \cdot 10^{-13}$ and $3.4 \cdot 10^{-12}$ $cm^3\ s^{-1}$(298 K, 1 atm)	2		a	1		a	1		a
HC5: Alkanes with OH rate constant between $3.4 \cdot 10^{-12}$ and $6.8 \cdot 10^{-12}$ $cm^3\ s^{-1}$(298 K, 1 atm)	1		a	0.5		a	0		a
HC8: Alkanes with OH rate constant greater than $6.8 \cdot 10^{-12}$ $cm^3\ s^{-1}$(298 K, 1 atm)	0.1		a	0		a	0		a
C_2H_4	1		a	0.5		a	0.1		a
OLT: Terminal alkenes	0.1		a	0.1		a	0.1		a
Isoprene	0.1	0	a	0.1	1	a	0.1	0	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	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_3OOH	0.01		a	0.01		a		0.01	a
OP2: Higher organic peroxides	0.01		a	0.01		a		0.01	a
$CH_3C(O)OOH$	0.001		a	0.001		a		0.001	a
CH_3OH	5		a	2		f		0.8	g
EtOH	1		c	0.24		f		$2.4 \cdot 10^{-3}$	h
Aqueous Phase species [M]									
$O_{2(aq)}$	$3 \cdot 10^{-4}$		b	$3 \cdot 10^{-4}$		b	$3 \cdot 10^{-4}$		b
OH^-	$3.16 \cdot 10^{-10}$			$3.16 \cdot 10^{-10}$			$1.6 \cdot 10^{-9}$		
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^+	$2.5 \cdot 10^{-7}$	0	d	$2.5 \cdot 10^{-8}$	0	d	$1 \cdot 10^{-9}$	0	d
Cu^{2+}	0	$2.5 \cdot 10^{-7}$		0	$2.5 \cdot 10^{-8}$		0	$1 \cdot 10^{-9}$	
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
$C_2O_4^{2-}$	$5 \cdot 10^{-6}$		k	$5 \cdot 10^{-7}$		k	$5 \cdot 10^{-8}$		k

Constant concentrations
during simulation time

$H_2O_{(g)}$	$2 \cdot 10^7$	$3 \cdot 10^7$	$3 \cdot 10^7$
$O_{2(g)}$	$2 \cdot 10^8$	$2 \cdot 10^8$	$2 \cdot 10^8$
$N_{2(g)}$	$7.8 \cdot 10^8$	$7.8 \cdot 10^8$	$7.8 \cdot 10^8$
$H_2O_{(aq)}$	55.5	55.5	55.5

[*)] only the changed values are noted in the column '2nd data set'; [a] Zimmermann and Poppe, 1996; [b] Graedel and Weschler, 1981; [c] Saxena and Hildemann, 1996; [d] Matthijsen and Builtjes, 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] $[C_2O_4]^{2-} = [Fe^{3+}]$, Sedlak and Hoigné, 1992, [l] Rohrer and Brüning, 1992

<u>Table 2:</u> Emissions and Depositions

<u>Table 2a:</u> Emissions

$[cm^{-3}\ s^{-1}] \cdot (10^5 cm$ height of layer$) = [cm^{-2}\ s^{-1}]$

	urban		remote		marine	
	1^{st} data set	2^{nd} data set	1^{st} data set	2^{nd} data set	1^{st} data set	2^{nd} data set
NO	$1.01 \cdot 10^7$		$2.86 \cdot 10^5$		$2.8 \cdot 10^4$	
CO	$8.99 \cdot 10^7$		$3.7 \cdot 10^6$		$8.53 \cdot 10^5$	
NH_3	$3.03 \cdot 10^6$		$9.06 \cdot 10^5$		$4.57 \cdot 10^5$	
SO_2	$3.27 \cdot 10^7$	$3.27 \cdot 10^6$	$2.91 \cdot 10^5$		$7.92 \cdot 10^4$	
HCHO	$2.58 \cdot 10^5$		3028		17.8	
ethane (ETH)	$1.54 \cdot 10^6$		$1.5 \cdot 10^4$		8.91	
HC3: Alkanes with OH rate constant between $2.7 \cdot 10^{-13}$ and $3.4 \cdot 10^{-12}\ cm^3\ s^{-1}$(298 K, 1 atm)	$2.76 \cdot 10^6$		$1.53 \cdot 10^4$		1.73	
HC5: Alkanes with OH rate constant between $3.4 \cdot 10^{-12}$ and $6.8 \cdot 10^{-12}\ cm^3\ s^{-1}$(298 K, 1 atm)	$4.9 \cdot 10^6$		$6.31 \cdot 10^4$		2.653	0
HC8: Alkanes with OH rate constant greater than $6.8 \cdot 10^{-12}\ cm^3\ s^{-1}$(298 K, 1 atm)	$3.19 \cdot 10^6$		$4.044 \cdot 10^4$		11.72	0
ethene (OL2)	$2.61 \cdot 10^6$		$4.54 \cdot 10^4$		45.0	
terminale alkenes (OLT)	$4.94 \cdot 10^5$		7950		7.28	0
dienes (DIEN)	$1.24 \cdot 10^6$		$1.55 \cdot 10^4$		11.7	
isoprene (ISO)	0	$1.54 \cdot 10^5$	0	$1.5 \cdot 10^6$		
TOL: Toluene and less reactive aromatics	$1.7 \cdot 10^6$		$2.108 \cdot 10^4$		5.81	
CSL: Cresol and other OH-substituted aromatics	$1.82 \cdot 10^6$		$2.88 \cdot 10^4$		7.78	0
XYL: Xylene and more reactive aromatics	$9.88 \cdot 10^5$		$1.13 \cdot 10^4$		0.721	0
acetaldehyde and higher aldehydes	$5.93 \cdot 10^5$		3171		10.41	
ketones (KET)	$9.9 \cdot 10^5$		8920		1.59	
CH_3COOH	$8.44 \cdot 10^4$		3350		810	
CH_3OH	$1.16 \cdot 10^6$		$1.07 \cdot 10^4$		0.59	
Ethanol	$4.03 \cdot 10^6$		3736		0.415	
α-Pinene (API)	$1.88 \cdot 10^5$	$1.93 \cdot 10^4$	$1.93 \cdot 10^4$	$1.88 \cdot 10^5$	8987	0
Limonene (LIM)	$1.88 \cdot 10^5$	$1.93 \cdot 10^4$	$1.93 \cdot 10^4$	$1.88 \cdot 10^5$	8987	0

Anthropogenic emissions from the EDGAR 1°-1° database of Olivier *et al.*, 1996, biogenic emissions from the global database of Guenther *et al.*, 1995. From these the maximum, median and minimum values for each species was calculated and used for the emission rates for the urban, rural and marine scenarios, respectively. Moreover, it must be noted that for certain species, such as isoprene, the estimates used in the marine case were set to zero. Dry deposition velocities for the most important gas phase species were taken from Ganzeveld *et al.,* 1998.

Table 2b: Depositions

[cm s^{-1}] / (10^5 cm height of layer) = [s^{-1}]

	urban = remote	**marine**
NO_2	$4 \cdot 10^{-6}$	$1 \cdot 10^{-6}$
HNO_3	$2 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
N_2O_5	$2 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
H_2O_2	$1 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
CO	$1 \cdot 10^{-6}$	$1 \cdot 10^{-6}$
O_3	$4 \cdot 10^{-6}$	$4 \cdot 10^{-7}$
HCl	$1 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
NH_3	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
SO_2	$1 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
H_2SO_4	$2 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
HCHO	$1 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
CH_3OOH	$5 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
HCOOH	$1 \cdot 10^{-5}$	$5 \cdot 10^{-6}$
CH_3OH	$1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
EtOH	$5 \cdot 10^{-6}$	$5 \cdot 10^{-6}$
HOBr	$2 \cdot 10^{-6}$	$2 \cdot 10^{-6}$
HOCl	$2 \cdot 10^{-6}$	$2 \cdot 10^{-6}$

Table 3: **Uptake Parameters**

Table 3a: **Henry's Law Constants**

red.	No 2.4	No. 2.3	Species	$K_{H\ 298}$, M atm^{-1}	ΔH / R, K	References	comment
	1	1	CO_2	*$3.11 \cdot 10^{-2}$* **$3.1 \cdot 10^{-2}$**	-2423	Chameides, 1984	
	2	2	HCl	1.10	-2020	Marsh and McElroy, 1985	
	3	3	NH_3	60.7	-3920	Clegg and Brimblecombe, 1990	
	4	4	O_3	$1.14 \cdot 10^{-2}$	-2300	Kosak-Channing and Helz, 1983	
	5	5	HO_2	$9 \cdot 10^3$		Weinstein-Lloyd and Schwartz, 1991	
	6	6	OH	25	-5280	Kläning *et al*., 1985b National Bureau of Standards, 1971	
	7	7	H_2O_2	$1.02 \cdot 10^5$	-6340	Lind and Kok, 1994	
	8	8	HNO_3	$2.1 \cdot 10^5$	-8700	Lelieveld and Crutzen, 1991	
	9	9	NO_3	0.6		Rudich *et al*., 1996	
	10	10	N_2O_5	1.4		*estimated equal as N_2O_4* **Schwartz and White, 1983**	value for N_2O_5 available
	11	11	NO_2	$1.2 \cdot 10^{-2}$	-1263	Schwartz and White, 1982	
	12	12	HNO_2	49	-4880	Park and Lee, 1988	
	13	13	HNO_4	*$1.0 \cdot 10^5$* $3 \cdot 10^4$		mean value from Möller and Mauersberger, 1992; Amels, 1996; Jacob *et al*, 1989 and Regimbal and Mozurkewich, 1997	*$K_H(HNO_4) = K_H(H_2O_2)$* **several measurements available**
	14	14	SO_2	1.24	-3247	Beilke and Gravenhorst, 1978	
	15	15	HCHO	*$3 \cdot 10^3$* 2.5	-7216	Betterton and Hoffmann, 1988a	physical solubility, not effective Henry's Law Constant
	16	16	CH_3OOH	*6* **310**	-5607	*Jacob, 1986* **Lind and Kok, 1994**	measurement, not estimate
*	17	17	$CH_3C(O)OOH$	669	-5890	Lind and Kok, 1994	
	18	18	CH_3OH	220	-5390	Betterton, 1992	
	19	19	C_2H_5OH	190	-6290	Betterton, 1992	
	20	20	CH_3CHO	*11.4* 4.8	-6254	Betterton and Hoffmann, 1988a	physical solubility, not effective Henry's Law Constant
	21	21	HCOOH	5530	-5630	Khan and Brimblecombe, 1992	
	22	22	CH_3COOH	5500	-5890	Khan and Brimblecombe, 1992	
	23	23	CH_3O_2	*6* 310	-5607	*Jacob, 1986* $K_H(CH_3O_2) = K_H(CH_3OOH)$	

	24	24	ETHP	*6*	-87	*$K_H(CH_3O_2) = K_H(ETHP)$*	better estimate
				340		estimated equal as CH_3CH_2OOH	O'Sullivan et al., 1996
	25	25	Cl_2	$9.15 \cdot 10^{-2}$	20.7	Wilhelm *et al.*, 1977	
	26	26	Br_2	0.758	31.6	Loomis, 1928	
	27	27	H_2SO_4	*$2.1 \cdot 10^{5}$*		$K_H(H_2SO_4) = K_H^{eff}(MSA)/K_A(MSA)$	better estimate
				$8.7 \cdot 10^{11}$		Brimblecombe and Clegg, 1988	
						$K_H(H_2SO_4) = K_H(HNO_3)$	
	28	28	ACO_3	669	*1263*	$K_H(ACO_3) = K_H(CH_3C(O)OOH)$	
					-5893		
	29		GLY	1.4		Betterton and Hoffmann, 1988a	
	30		O_2	$1.3 \cdot 10^{-3}$	-1700	Loomis, 1928	
	31		$ClNO_2$	0.024		Behnke *et al.*, 1997	
	32		$BrNO_2$	0.3		Frenzel *et al.*, 1998	
	33		BrCl	0.94		Bartlett and Margerum, 1998	
	34		NO	$1.2 \cdot 10^{-2}$	-1263		

Table 3 b: Mass accommodation coefficients and Gas Phase Diffusion Coefficients

red.	No 2.4	No 2.3	Species	α	References	α (288 K)	D_g [10^5 m^2 s^{-1}]	References	comment
	1	1	CO_2	$2 \cdot 10^{-4}$	estimated	$1.5 \cdot 10^{-4}$	1.55	McElroy, 1997	
	2	2	HCl	0.064	Davidovits *et al.*, 1995	0.1158	1.89	Marsh and McElroy, 1985	
	3	3	NH_3	0.04	Bongartz, 1995	0.091	2.3	Ponche, 1993	
	4	4	O_3	$5 \cdot 10^{-2}$	Mirabel, 1996	0.1	1.48	Schwartz, 1986	
	5	5	HO_2	0.01	Hanson, 1992	0.01	1.04	Hanson, 1992	
	6	6	OH	0.05	estimated	0.05	1.53	Hanson, 1992	
	7	7	H_2O_2	0.11	Davidovits *et al.*, 1995	0.1532	1.46	McElroy, 1997	
	8	8	HNO_3	0.054	Davidovits *et al.*, 1995	0.0868	1.32	Kirchner, 1990	
	9	9	NO_3	$4 \cdot 10^{-3}$	Kirchner, 1990	$4 \cdot 10^{-3}$	1.00	Thomas, 1998	
					Rudich, 1996				
	10	10	N_2O_5	$3.7 \cdot 10^{-3}$	George et al., 1994	0.018	1.10	Kirchner, 1990	
	11	11	NO_2	$1.5 \cdot 10^{-3}$	estimated	0.0015	1.92	Ponche, 1993	
	12	12	HNO_2	0.5	Bongartz, 1995	0.5	1.30	Kirchner, 1990	
	13	13	HO_2NO_2	0.1	Jacob, 1986	0.1	1.30	Schweitzer, 1998	
	14	14	SO_2	$3.5 \cdot 10^{-2}$	Tang and Lee, 1987	0.11	1.28	McElroy, 1997	
					Gardner, 1987				
	15	15	HCHO	0.02	estimated	0.02	1.64	Fuller, 1986 [a)]	
	16	16	CH_3OOH	$3.8 \cdot 10^{-3}$	Davidovits *et al.*, 1995	$6.758 \cdot 10^{-3}$	1.31	Fuller, 1986 [a)]	

*	17	17	$CH_3C(O)OOH$	0.019	$\alpha_{17} = \alpha_{31}$	0.019	1.02	Fuller, 1986 [a)]	
	18	18	CH_3OH	$1.5 \cdot 10^{-2}$	Davidovits *et al.*, 1995	0.0271	1.16	Schwartz, 1986	
	19	19	C_2H_5OH	$8.2{\cdot}10^{-3}$	Davidovits *et al.*, 1995	0.0176	0.95	Schwartz, 1986	
	20	20	CH_3CHO	0.03	estimated	0.03	1.22	Fuller, 1986 [a)]	
	21	21	HCOOH	0.012	Davidovits *et al.*, 1995	0.0229	1.53	Schwartz, 1986	
	22	22	CH_3COOH	0.019	Davidovits *et al.*, 1995	0.0322	1.24	Schwartz, 1986	
	23	23	CH_3O_2	$3.8{\cdot}10^{-3}$	$\alpha = \alpha_{CH3OOH}$	$6.7581{\cdot}10^{-3}$	1.35	Fuller, 1986 [a)]	
	24	24	ETHP	$8.2 \cdot 10^{-3}$	estimated	$8.2 \cdot 10^{-3}$	1.08	Fuller, 1986 [a)]	
	25	25	Cl_2	0.03	estimated	0.08	1.28	Schwartz, 1986	
	26	26	Br_2	0.03	estimated	0.08	1.00	Schwartz, 1986	
	27	27	H_2SO_4	0.07	Davidovits *et al.*, 1995	0.12	1.30	Schwartz, 1986	
	28	28	ACO_3	0.019	$\alpha = \alpha_{CH3COOH}$	0.019	1.0	Fuller, 1986 [a)]	
	29		GLY	0.023		0.023	1.15	Fuller, 1986 [a)]	also GLY-chem. in aq. phase considered
	30		O_2	0.1	estimated	0.01	1.12	Fuller, 1986 [a)]	no initial conc. for O_2 in the aq. phase
	31		$ClNO_2$	0.01	Schweitzer, 1998	0.01	1.44	Fuller, 1986 [a)]	formed in the aq. phase
	32		$BrNO_2$	0.01	Schweitzer, 1998	0.01	1.44	Fuller, 1986 [a)]	formed in the aq. phase
	33		BrCl	0.33	Katrib *et al.*, ?	0.33	1.19	Fuller, 1986 [a)]	formed in the aq. phase
	34		NO	0.001		0.001	2.24		formed in the aq. phase
		29	*CH_4*	$5{\cdot}10^{-5}$	estimated		1.41	Fuller, 1986 [a)]	removed because no further processes in the aqueous phase
		30	*C_2H_6*	$1{\cdot}10^{-4}$	estimated		0.95	Fuller, 1986 [a)]	"
		31	*C_2H_4*	$1{\cdot}10^{-4}$	estimated		1.01	Fuller, 1986 [a)]	"
		32	*PAN*	0.019	estimated		0.63	Fuller, 1986 [a)]	"
		33	*OP2*	0.01	estimated		0.76	Fuller, 1986 [a)]	"
		34	*OL2P*	$8.2{\cdot}10^{-3}$	estimated		0.82	Fuller, 1986 [a)]	"

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

Table 4: HO_x- and Transition metal ion (TMI)-Chemistry

red	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Reference	comment
	1	1	$H_2O_2 + Fe^{2+} \rightarrow OH + OH^- + Fe^{3+}$	*76*		*Walling, 1975*	
				50		Barb *et al.*, 1950	several studies confirm this value
*	2		$Mn(OH)^{2+} + H_2O_2 \rightarrow MnO_2^+ + H^+ + H_2O$	$2.8 \cdot 10^3$		Jacobsen *et al.*,1997	new data available (MnO_2^+)
*	3		$Mn^{4+} + H_2O_2 \rightarrow Mn^{2+} + 2\ H^+ + O_2$	$1 \cdot 10^6$		Jacobsen *et al.*, 1997	new data available
	4	2	$H_2O_2 + Cu^+ \rightarrow OH + OH^- + Cu^{2+}$	$7.0 \cdot 10^3$		Berdnikov, 1973	
*	5	3	$H_2O_2 + Mn^{3+} \rightarrow HO_2 + H^+ + Mn^{2+}$	$7.3{\cdot}10^4$		Davies *et al.,* 1968	

	6	4	$O_2^- + Fe^{3+} \rightarrow O_2 + Fe^{2+}$	$1.5 \cdot 10^8$		Rush and Bielski, 1985	
	7	5	$HO_2 + [Fe(OH)]^{2+} \rightarrow Fe^{2+} + O_2 + H_2O$	$1.3 \cdot 10^5$		Ziajka *et al.*, 1994	
	8	6	$O_2^- + [Fe(OH)]^{2+} \rightarrow O_2 + Fe^{2+} + OH^-$	$1.5 \cdot 10^8$		Rush and Bielski, 1985	
*	9	7	$O_2^- + [Fe(OH)_2]^+ \rightarrow O_2 + Fe^{2+} + 2\ OH^-$	$1.5 \cdot 10^8$		Rush and Bielski, 1985	
	10	8	$O_2^- + Fe^{2+}\ (+ 2\ H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.0 \cdot 10^7$		Rush and Bielski, 1985	
	11	9	$HO_2 + Fe^{2+}\ (+ H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.2 \cdot 10^6$	5050	Jayson *et al.*, 1973b	
	12	10	$OH + Fe^{2+} \rightarrow [Fe(OH)]^{2+}$	$4.3 \cdot 10^8$	1100	Christensen and Sehested, 1981	
*	13		$MnO_2^+ + HO_2\ (+ H^+) \rightarrow Mn^{2+} + H_2O_2 + O_2$	$1 \cdot 10^7$		Jacobsen *et al.*, 1997	new data available (MnO_2^+)
*	14		$OH + Mn^{2+} \rightarrow OH^- + Mn^{3+}$	*$2.6 \cdot 10^7$*		*Baral et al., 1986*	new data available; consistent to other
				$2 \cdot 10^7$		Jacobsen *et al.*, 1997	(new) Mn reactions
	15	11	$O_2^- + Cu^+\ (+ 2\ H^+) \rightarrow H_2O_2 + Cu^{2+}$	*$9.4 \cdot 10^9$*		*von Piechowski et al., 1993*	measurement instead of computer
				$1 \cdot 10^{10}$		Rabani *et al.*, 1973	simulation
	16	12	$HO_2 + Cu^+\ (+ H^+) \rightarrow H_2O_2 + Cu^{2+}$	*$2.2 \cdot 10^9$*		Kozlov and Berdnikov, 1973	corrected value
				$3 \cdot 10^9$			
*	17	13	$OH + Cu^+ \rightarrow OH^- + Cu^{2+}$	$3 \cdot 10^9$		Goldstein *et al.*, 1992	
	18	14	$HO_2 + Cu^{2+} \rightarrow O_2 + Cu^+ + H^+$	*$1.2 \cdot 10^9$*		*Cabelli et al., 1987*	to be consistent to R19 (pH: 3-6.5;
				$1 \cdot 10^8$		Rabani *et al.*, 1973	former value: pH = 4.5)
	19	15	$O_2^- + Cu^{2+} \rightarrow O_2 + Cu^+$	*$1.1 \cdot 10^{10}$*		*Cabelli et al., 1987*	"
				$8 \cdot 10^9$		Rabani *et al.*, 1973	
	20	16	$Fe^{3+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+}$	*$3 \cdot 10^7$*		*Sedlak and Hoigné, 1993*	measurement instead of estimate
				$1.3 \cdot 10^7$		Buxton *et al.*, 1995-	
	21	17	$[Fe(OH)]^{2+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + OH^-$	*$3 \cdot 10^7$*		*Sedlak and Hoigné, 1993*	measurement instead of estimate
				$1.3 \cdot 10^7$		Buxton *et al.*, 1995	
*	22	18	$[Fe(OH)_2]^+ + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + 2\ OH^-$	*$3 \cdot 10^7$*		*Sedlak and Hoigné, 1993*	measurement instead of estimate
				$1.3 \cdot 10^7$		Buxton *et al.*, 1995	
	23	19	$Fe^{2+} + Mn^{3+} \rightarrow Fe^{3+} + Mn^{2+}$	*$1.5 \cdot 10^4$*		Diebler and Sutin, 1964	
				$1.6 \cdot 10^4$			
	24	20	$O_3 + O_2^- \xrightarrow{H^+} \mathit{2\ O_2 + OH} \rightarrow O_3^- + O_2$	$1.5 \cdot 10^9$	2200	Sehested *et al.*, 1983	split into elementary steps
						Hesper and Herrmann, 2000	
	25		$HO_3 \rightarrow OH + O_2$	330	4500	Bühler *et al.*, 1984	split into elementary steps
						Hesper and Herrmann, 2000	
*	26	21	$HO_2 + HO_2 \rightarrow O_2 + H_2O_2$	$8.3 \cdot 10^5$	2720	Bielski *et al.*, 1985	
*	27	22	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2 + O_2$	$9.7 \cdot 10^7$	1060	Bielski *et al.*, 1985	
*	28	23	$HO_2 + OH \rightarrow H_2O + O_2$	$1.0 \cdot 10^{10}$		Elliot and Buxton, 1992	
*	29	24	$O_2^- + OH \rightarrow OH^- + O_2$	$1.1 \cdot 10^{10}$	2120	Christensen *et al.*, 1989	
	30	25	$H_2O_2 + OH \rightarrow HO_2 + H_2O$	$3.0 \cdot 10^7$	1680	Christensen *et al.*, 1982	

*	31	26	$CH_3OOH + OH \rightarrow CH_3O_2 + H_2O$	*3·10^7* 2.4·10^7	1680	31/32: Sum is equal as before	consideration of another reaction pathway
*	32		$CH_3OOH + OH \rightarrow \mathbf{HO_2 + HCOOH}$	$6.0 \cdot 10^6$	1680	branching ratio 0.8 : 0.2 (correlation for H abstractions)	
	33	27	$HSO_3^- + OH \rightarrow H_2O + SO_3^-$	$2.7 \cdot 10^9$		Buxton *et al.*, 1996a	
*	34	28	$SO_3^{2-} + OH \rightarrow OH^- + SO_3^-$	$4.6 \cdot 10^9$		Buxton *et al.*, 1996a	
*	35		$MnO_2^+ + MnO_2^+ \rightarrow 2\ Mn^{2+} + H_2O_2$	$6 \cdot 10^6$		Jacobsen *et al.*,1997	new data available (MnO_2^+)
	36		$Cu^+ + O_2 \rightarrow Cu^{2+} + O_2^-$	$4.6 \cdot 10^5$		Bjergbakke *et al.*, 1976	
	37		$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	$8.2 \cdot 10^5$		Logager *et al.*, 1992	new data available (FeO^{2+})
*	38		$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	$9.5 \cdot 10^3$	2766	Jacobsen *et al.*, 1998a)	"
*	39		$FeO^{2+} + H_2O \rightarrow Fe^{3+} + OH + OH^-$	$2.34 \cdot 10^{-4}$	4089	Jacobsen *et al.*, 1998a)	"
*	40		$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	$2.0 \cdot 10^6$		Jacobsen *et al.*, 1997a	"
*	41		$FeO^{2+} + OH \rightarrow Fe^{3+} + H_2O_2$	$1.0 \cdot 10^7$		Logager *et al.*, 1992	"
*	42		$FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$	$1.1 \cdot 10^4$	4150	Jacobsen *et al.*, 1998b)	"
*	43		$FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH$	$2.5 \cdot 10^5$		Jacobsen *et al.*, 1998b)	"
	44		$FeO^{2+} + Cl^- \xrightarrow{H^+} Fe^{3+} + ClOH^-$	100		Jacobsen *et al.*, 1998b)	"
*	45		$FeO^{2+} + Mn^{2+} \xrightarrow{2H^+} Mn^{3+} + Fe^{3+} + H_2O$	$1.0 \cdot 10^4$	2562	Jacobsen *et al.*, 1998b)	"
*	46		$FeO^{2+} + HCOOH \xrightarrow{H^+} Fe^{3+} + COOH + H_2O$	160	2680	Jacobsen *et al.*, 1998b)	"
*	47		$FeO^{2+} + HCOO^- \rightarrow Fe^{3+} + COOH + OH^-$	$3 \cdot 10^5$		Jacobsen *et al.*, 1998b)	"
*	48		$FeO^{2+} + C_2H_5OH \rightarrow Fe^{3+} + CH_3CHOH + OH^-$	$2.5 \cdot 10^3$		Jacobsen *et al.*, 1998b)	"
*	49		$FeO^{2+} + CH_2(OH)_2 \rightarrow Fe^{3+} + OH^- + CH(OH)_2$	400	5352	Jacobsen *et al.*, 1998b)	"
*	50		$FeO^{2+} + NO_2^- \xrightarrow{H^+} Fe^{3+} + NO_2 + OH^-$	$1 \cdot 10^5$		Jacobsen *et al.*, 1998b)	"
	51		$FeO^{2+} + Fe^{2+} \rightarrow 2\ Fe^{3+} + 2$ OH-	$7.2 \cdot 10^4$	842	Jacobsen *et al.*, 1997a)	"
*	52		$FeO^{2+} + Fe^{2+} \xrightarrow{2H_2O^+} FeOH_2Fe^{4+} + 2\ OH^-$	$1.8 \cdot 10^4$	5052	Jacobsen *et al.*, 1997a)	"
*	53		$FeOH_2Fe^{4+} + H^+ \xrightarrow{H^+} 2\ Fe^{3+} + H_2O$	1.95	5653	Jacobsen *et al.*, 1997a)	"
*	54		$FeOH_2Fe^{4+} \rightarrow 2\ Fe^{3+} + 2\ OH^-$	0.49	8780	Jacobsen *et al.*, 1997a)	"
*	55		$MnO^{2+} + Mn^{2+} \xrightarrow{2H^+} 2\ Mn^{3+} + H_2O$	$1 \cdot 10^5$		Jacobsen *et al.*, 1998a)	new data available
*	56		$Mn^{2+} + O_3 \rightarrow MnO^{2+} + O_2$	$1.65 \cdot 10^3$		Jacobsen *et al.*, 1998a)	new data available
*	57		$Cu^+ + O_3 \xrightarrow{H^+} Cu^{2+} + OH + O_2$	$3 \cdot 10^7$		Hoigné and Bühler, 1996	new data available
*	58		$OH + O_3 \rightarrow O_2 + HO_2$	$1 \cdot 10^8$		Sehested *et al.*, 1984	additional sink for OH/O_3
*	59		$O^3P + O_2 \rightarrow O_3$	$4 \cdot 10^9$		Kläning *et al.*, 1984	sink for O^3P (NO_3 photolysis)

<u>Table 5:</u> Nitrogen-Chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Reference	comment
	60		$N_2O_5 \rightarrow NO_2^+ + NO_3^-$	$1{\cdot}10^9$		estimated	correct formulation
	61		$NO_2^+ + H_2O \rightarrow NO_3^- + 2H^+$	$8.9{\cdot}10^7$		Behnke *et al.*, 1997	correct formulation
		29	*$N_2O_5 + H_2O \rightarrow 2\ H^+ + 2\ NO_3^-$*	*$5 \cdot 10^9$*		*estimated*	wrong formulation
*	62	30	$NO_3 + OH^- \rightarrow NO_3^- + OH$	$9.4 \cdot 10^7$	2700	Exner *et al.*, 1992	
*	63	31	$NO_3 + Fe^{2+} \rightarrow NO_3^- + Fe^{3+}$	$8 \cdot 10^6$		Pikaev *et al.*, 1974	
*	64	32	$NO_3 + Mn^{2+} \rightarrow NO_3^- + Mn^{3+}$	$1.1 \cdot 10^6$		Neta and Huie, 1986	
*	65	33	$NO_3 + H_2O_2 \rightarrow NO_3^- + H^+ + HO_2$	$4.9 \cdot 10^6$	2000	Herrmann *et al.*, 1994	
*	66	34	$NO_3 + CH_3OOH \rightarrow NO_3^- + H^+ + CH_3O_2$	$4.9 \cdot 10^6$	2000	$k = k_{H2O2}$	
*	67	35	$NO_3 + HO_2 \rightarrow NO_3^- + H^+ + O_2$	$3.0 \cdot 10^9$		Sehested *et al.*, 1994	
*	68	36	$NO_3 + O_2^- \rightarrow NO_3^- + O_2$	$3.0 \cdot 10^9$		$k = k_{HO2}$	
	69	37	$NO_3 + HSO_3^- \rightarrow NO_3^- + H^+ + SO_3^-$	$1.3 \cdot 10^9$	2000	Exner *et al.*, 1992	
*	70	38	$NO_3 + SO_3^{2-} \rightarrow NO_3^- + SO_3^-$	$3.0 \cdot 10^8$		Exner *et al.*, 1992	
*	71	39	$NO_3 + HSO_4^- \rightarrow NO_3^- + H^+ + SO_4^-$	$2.6 \cdot 10^5$		Raabe, 1996	
	72	40	$NO_3 + SO_4^{2-} \rightarrow NO_3^- + SO_4^-$	*$5.6{\cdot}10^3$* $1{\cdot} 10^5$		Logager *et al.*, 1993	corrected value
*	73	41	*$NO_2 + OH \rightarrow NO_3^- + H^+$* **$NO_2 + OH \rightarrow HOONO$**	$1.2 \cdot 10^{10}$		Wagner *et al.*, 1980	correct product; in 2.3 for simplification lumped to HNO_3
*	74	42	$NO_2 + O_2^- \rightarrow NO_2^- + O_2$	$1 \cdot 10^8$		Warneck and Wurzinger, 1988	
*	75	43	$NO_2 + NO_2\ (+ H_2O) \rightarrow HNO_2 + NO_3^- + H^+$	$8.4 \cdot 10^7$	-2900	Park and Lee, 1988	
	76	44	$O_2NO_2^- \rightarrow NO_2^- + O_2$	1		Løgager and Sehested, 1993	
*	77	45	$NO_2^- + OH \rightarrow NO_2 + OH^-$	*$1.1{\cdot}10^{10}$* $9.1 \cdot 10^9$		Barker *et al.*, 1970	measurement in more alkaline solution
*	78	46	$NO_2^- + SO_4^- \rightarrow SO_4^{2-} + NO_2$	$7.2 \cdot 10^8$		Reese, 1997	
*	79	47	$NO_2^- + NO_3 \rightarrow NO_3^- + NO_2$	$1.4 \cdot 10^9$	0	Herrmann and Zellner, 1998	
*	80	48	$NO_2^- + Cl_2^- \rightarrow 2\ Cl^- + NO_2$	$6 \cdot 10^7$		Jacobi, 1996	
*	81	49	$NO_2^- + Br_2^- \rightarrow 2\ Br^- + NO_2$	$1.2 \cdot 10^7$	1720	*Shoute et al., 1991* Jacobi, 1996	
*	82	50	$NO_2^- + CO_3^- \rightarrow CO_3^{2-} + NO_2$	$6.6 \cdot 10^5$	850	Huie *et al.*, 1991a	
*	83	51	$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	$5 \cdot 10^5$	*7000* 6900	Damschen and Martin, 1983	corrected value

	84	52	$HNO_2 + OH \rightarrow NO_2 + H_2O$	*1·10^9^* $\mathit{1{\cdot}10^{9}}$ $1.1 \cdot 10^{10}$		*Rettich, 1978* Barker *et al.*, 1970	measurement in more alkaline solution
	85		$NO_2^+ + Cl^- \rightarrow ClNO_2$	$1{\cdot}10^{10}$		Chr. George, pers. comm., 1999	considering of XNO_2 chemistry
	86		$NO_2^+ + Br^- \rightarrow BrNO_2$	$1{\cdot}10^{10}$		Chr. George, pers. comm., 1999	"
	87		$ClNO_2 + Br^- \rightarrow NO_2^- + BrCl$	$5{\cdot}10^{6}$		Chr. George, pers. comm., 1999	"
	88		$BrNO_2 + Br^- \rightarrow NO_2^- + Br_2$	$2.55{\cdot}10^{4}$		Chr. George, pers. comm., 1999	"
	89		$BrNO_2 + Cl^- \rightarrow NO_2^- + BrCl$	10		Chr. George, pers. comm., 1999	"

<u>Table 6:</u> Sulfur-Chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\,s^{-1}$	E_a / R, K	Reference	comment
	90	53	$HMS^- + OH \rightarrow$ *$H_2O + HO_2 + HCOOH + HSO_3^-$* $H_2O + CHOHSO_3^-$	$3{\cdot}10^{8}$		Barlow et al., 1997b)	correct products; split into elementary steps
*	91	54	$HMS^- + SO_4^- \rightarrow SO_4^{2-}$ *$+ H^+ + HCHO + SO_3^-$* $SO_4^{2-} + OHCH_2SO_3$	*$2.8{\cdot}10^{6}$* **$1.3{\cdot}10^{6}$**		Barlow et al., 1997b)	"
*	92	55	$HMS^- + NO_3 \rightarrow$ *$NO_3^- + H^+ + HCHO + SO_3^-$* $NO_3^- + OHCH_2SO_3$	$4.2{\cdot}10^{6}$		Herrmann et al., 1996a) Barlow et al., 1997b)	"
*	93	56	$HMS^- + Cl_2^- \rightarrow$ *$2\,Cl^- + H^+ + HCHO + SO_3^-$* $2\,Cl^- + OHCH_2SO_3$	$5.0{\cdot}10^{5}$		Jacobi, 1996 Barlow et al., 1997b)	"
*	94	57	$HMS^- + Br_2^- \rightarrow$ *$2\,Br^- + H^+ + HCHO + SO_3^-$* $2\,Br^- + OHCH_2SO_3$	$5.0{\cdot}10^{4}$		estimated as $k = 0.1k(Cl_2^-)$	"
*	95		$OHCH_2SO_3 \rightarrow SO_3 + CH_2OH$	$1{\cdot}10^{5}$		estimated	sink for $OHCH_2SO_3$
*	96		$SO_3 + H_2O \rightarrow SO_4^{2-} + 2\,H^+$	$1{\cdot}10^{10}$		estimated as diffusion controlled	sink for SO_3
	97		$CHOSOH_3^- + O_2 \rightarrow O_2CHOHSO_3^-$	$2.6 \cdot 10^{9}$		Barlow *et al.*, 1997b	split into elementary steps; consideration of side reactions
	98		$O_2CHOHSO_3^- \rightarrow HO_2 + CHOSO_3^-$	$1.7 \cdot 10^{4}$		Barlow *et al.*, 1997b	"
	99		$O_2CHOHSO_3^- \rightarrow O_2CHO + HSO_3^-$	$7.0{\cdot}\,10^{3}$		Barlow *et al.*, 1997b	"
	100		$CHOSO_3^- + H_2O \rightarrow HSO_3^- + HCOOH$	$1.26{\cdot}10^{-2}$		Buxton *et al.*, 1997	"
	101		$O_2CHO + H_2O \rightarrow HCOOH + HO2$	44.32		Barlow *et al.*, 1997b	"
*	102		$CHOHSO_3^{2-} + O_2 \rightarrow CHOHSO_3^- + O_2^-$	$1.6 \cdot 10^{9}$		Barlow *et al.*, 1997b	"
	103	58	$HSO_3^- + H_2O_2 + H^+ \rightarrow SO_4^{2-} + H_2O + 2\,H^+$	*$6.9 \cdot 10^{7}$* **$7.2 \cdot 10^{7}$**	4000	*Zellner et al., 1994* Lind *et al.*, 1987	to be consistent to 104/105
*	104	59	$HSO_3^- + CH_3OOH + H^+ \rightarrow SO_4^{2-} + 2\,H^+ + CH_3OH$	*$1.8{\cdot}\,10^{7}$* **$1.7 \cdot 10^{7}$**	3800	Lind *et al.*, 1987	corrected value
*	105	60	$HSO_3^- + CH_3C(O)OOH + H^+ \rightarrow SO_4^{2-} + 2\,H^+$ *+prod.–* **$+ CH_3COOH$**	*$4.8 \cdot 10^{7}$* $5.6 \cdot 10^{7}$	3990	Lind *et al.*, 1987	correct product; analogous to other HSO_3^- + ROOH
*	106	61	$SO_2 + O_3$ *$(+ H_2O)$* $\rightarrow HSO_4^- + O_2 + H^+$	$2.4 \cdot 10^{4}$		Hoffmann, 1986	

	107	62	$HSO_3^- + O_3 \rightarrow HSO_4^- + O_2$	$3.7 \cdot 10^5$	5530	Hoffmann, 1986	
	108	63	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	$1.5 \cdot 10^9$	5280	Hoffmann, 1986	
*	109	64	$[Fe(OH)]^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	*39*		Ziajka *et al.*, 1994	
				30			
	110	65	$Fe^{2+} + SO_5^- (+ H_2O) \rightarrow [Fe(OH)]^{2+} + HSO_5^-$	*$4.3 \cdot 10^7$*	5809	*Herrmann et al., 1996a*	T dependent value
				$2.65 \cdot 10^7$		Williams, 1996	
	111	66	$Fe^{2+} + HSO_5^- \rightarrow [Fe(OH)]^{2+} + SO_4^-$	$3 \cdot 10^4$		Ziajka *et al.*, 1994	
*	112		$Mn^{2+} + HSO_5^- \rightarrow SO_4^- + Mn^{3+} + OH^-$	$3 \cdot 10^4$		estimated equal as $k_{(Fe2+ + HSO5-)}$	completion of Mn chemistry
*	113	67	$Mn^{2+} + SO_5^- (+ H_2O) \rightarrow Mn^{3+} + HSO_5^- + OH^-$	*$4.6 \cdot 10^6$*		*Herrmann et al., 1996a*	to be consistent to R146
				$1 \cdot 10^{10}$		**Berglund et al., 1994**	
	114		$Fe^{2+} + SO_4^- (+ H_2O) \rightarrow [Fe(OH)]^{2+} + SO_4^{2-} + H^+$	*$3.5 \cdot 10^7$*		*Ziajka et al., 1994*	T dependent value
				$4.6 \cdot 10^9$	-2165	Buxton *et al.*, 1997	
*	115		$Fe^{2+} + S_2O_8^{2-} (+ H_2O) \rightarrow [Fe(OH)]^{2+} + SO_4^{2-}$	17		*Ziajka et al., 1994*	measurement instead of estimate
			$+ SO_4^{2-} + H^+$			Buxton *et al.*, 1997	
*	116	68	$SO_5^- + SO_5^- \rightarrow S_2O_8^{2-} + O_2$	*$1.8 \cdot 10^8$*	2600	*Herrmann et al., 1995*	new evidences about product ratio
				$4.8 \cdot 10^7$		Buxton *et al.*, 1997	
	117	69	$SO_5^- + SO_5^- \rightarrow 2\ SO_4^- + O_2$	*$7.2 \cdot 10^6$*	2600	*Herrmann et al., 1995*	"
				$2.2 \cdot 10^8$		Buxton *et al.*, 1997	
	118	70	$SO_5^- + HO_2 \rightarrow HSO_5^- + O_2$	$1.7 \cdot 10^9$		Buxton *et al.*, 1996b	correct product; split into elementary steps
			$\rightarrow SO_5O_2H^-$				
*	119		$SO_5^- + O_2^- (+ H^+) \rightarrow HSO_5^- + OH^- + O_2$	$1.7 \cdot 10^9$			
				$2.34 \cdot 10^8$		Buxton *et al.*, 1996a	
*	120		$SO_5O_2H^- + HSO_3^- \rightarrow 2\ SO_4^{2-} + 2\ H^+$	$3.0 \cdot 10^5$		Buxton *et al.*, 1997	split into elementary steps; sink reaction
*	121		$SO_5O_2^{2-} + HSO_3^- \rightarrow 2\ SO_4^{2-} + H^+$	$5.2 \cdot 10^6$		Buxton *et al.*, 1997	"
	122		$SO_5O_2^{2-} (+ H^+) \rightarrow HSO_5^- + O_2$	1200		Buxton *et al.*, 1997	"
	123	71	$SO_3^- + O_2 \rightarrow SO_5^-$	$2.5 \cdot 10^9$		Buxton *et al.*, 1996a	
*	124	72	$SO_5^- + HSO_3^- \rightarrow HSO_5^- + SO_3^-$	$8.6 \cdot 10^3$		Buxton *et al.*, 1996a	
*	125	73	$SO_5^- + HSO_3^- \rightarrow SO_4^{2-} + SO_4^- + H^+$	$3.6 \cdot 10^2$		Buxton *et al.*, 1996a	
*	126	74	$SO_5^- + SO_3^{2-} (+ H^+) \rightarrow HSO_5^- + SO_3^-$	$2.13 \cdot 10^5$		Buxton *et al.*, 1996a	
*	127	75	$SO_5^- + SO_3^{2-} \rightarrow SO_4^- + SO_4^{2-}$	$5.5 \cdot 10^5$		Buxton *et al.*, 1996a	
*	128	76	$OH + HSO_4^- \rightarrow H_2O + SO_4^-$	$3.5 \cdot 10^5$		Tang *et al.*, 1988	
*	129		$SO_4^- + SO_4^- \rightarrow S_2O_8^{2-}$	*$1.6 \cdot 10^8$*		*Herrmann et al., 1995a)*	T dependent value
				$6.1 \cdot 10^8$	840	Ervens, 1997	
*	130		$SO_4^- + HSO_3^- \rightarrow SO_4^{2-} + SO_3^- + H^+$	*$3.2 \cdot 10^8$*		*Reese, 1997*	
				$5.8 \cdot 10^8$		mean value of Reese, 1997; Wine *et al.*, 1989; Buxton *et al.*, 1996a	mean value of all available data
*	131		$SO_4^- + SO_3^{2-} \rightarrow SO_4^{2-} + SO_3^-$	*$3.2 \cdot 10^8$*	1200	*Reese, 1997*	

				$3.4 \cdot 10^{8}$		mean value of Reese, 1997; Wine *et al*., 1989., Buxton *et al*., 1996a	mean value of all available data
*		77	*$SO_4^- + Fe^{2+} \rightarrow [Fe(SO_4)]^+$*	*$3 \cdot 10^{8}$*		*McElroy and Waygood, 1990*	no evidence that rxn. takes place
*	132		$SO_4^- + Mn^{2+} \rightarrow SO_4^{2-} + Mn^{3+}$	*$2 \cdot 10^{7}$*		*Neta and Huie, 1987*	
				$1.4 \cdot 10^{7}$	4089	Buxton *et al*., 1996b	T dependent value
*	133		$SO_4^- + Cu^+ \rightarrow SO_4^{2-} + Cu^{2+}$	$3 \cdot 10^{8}$		estimated equal as $k_{(Fe2+ + SO4- \rightarrow FeSO4+)}$; McElroy and Waygood, 1990)	formulated analagous to Fe/ Mn chemistry
*	134	78	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	*$2.8 \cdot 10^{7}$*		*Reese, 1997*	mean value of all available data
				$1.7 \cdot 10^{7}$		mean value of Reese, 1997; Wine *et al.*, 1989; Maruthamutu and Neta, 1978	
*	135	79	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + H^+ + CH_3O_2$	*$2.8 \cdot 10^{7}$*		$k = k_{H2O2}$	equal as k_{H2O2}
				$1.7 \cdot 10^{7}$			
*	136	80	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+ + O_2$	$3.5 \cdot 10^{9}$		Jiang *et al*., 1992	
*	137	81	$SO_4^- + O_2^- \rightarrow SO_4^{2-} + O_2$	$3.5 \cdot 10^{9}$		$k_{HO2} = k_{O2-}$	
*	138	82	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	$5.0 \cdot 10^{4}$		Exner *et al*., 1992	
*	139	83	$SO_4^- + OH^- \rightarrow SO_4^{2-} + OH$	$1.4 \cdot 10^{7}$		Herrmann *et al*., 1995b	
	140	84	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	11	1110	Herrmann *et al*., 1995b	
	141	85	$HSO_5^- + HSO_3^- + H^+ \rightarrow 2\ SO_4^{2-} + 3\ H^+$	$7.14 \cdot 10^{6}$		Betterton and Hoffmann, 1988b	
*	142	86	$HSO_5^- + SO_3^{2-} + H^+ \rightarrow 2\ SO_4^{2-} + 2\ H^+$	$7.14 \cdot 10^{6}$		Betterton and Hoffmann, 1988b	
*	143	87	$HSO_5^- + OH \rightarrow SO_5^- + H_2O$	$1.7 \cdot 10^{7}$		Maruthamuthu and Neta, 1977	
*	144	88	$HNO_4 + HSO_3^- \rightarrow HSO_4^- + NO_3^- + H^+$	$3.3 \cdot 10^{5}$		Amels *et al*., 1996	
*	145		$OH + SO_4^- \rightarrow HSO_5^-$	$1.0 \cdot 10^{10}$		Wilhelm *et al*., 1977	new sink for SO_4^-/source HSO_5^-
*	146		$MnHSO_3^+ + Mn^{3+} \rightarrow 2\ Mn^{2+} + SO_3^- + H^+$	$1.3 \cdot 10^{6}$		Berglund *et al*., 1994	
*	147		$SO_5^- + HC_2O_4^- \rightarrow HSO_5^- + C_2O_4^-$	$5 \cdot 10^{3}$		Herrmann *et al*., 2000	consideration of C_2-difunctional
*	148		$SO_5^- + C_2O_4^{2-} \rightarrow HSO_5^- + C_2O_4^-$	$1 \cdot 10^{4}$		Herrmann *et al*., 2000	compounds
*	149		$SO_5^- + CH(OH)_2CH(OH)_2 \rightarrow HSO_5^- + C(OH)_2CH(OH)_2$	$5 \cdot 10^{5}$		Herrmann *et al*., 2000	"

Table 7: Organic Chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n} s^{-1}$	E_a / R, K	Reference	comment
	150	89	$CH_3OH + OH$ *$(+O_2) \rightarrow H_2O + HO_2 + HCHO$* $\rightarrow H_2O + CH_2OH$	$1.0 \cdot 10^9$	580	Elliot and McCracken, 1989	split into elementary steps
*	151	90	$CH_3OH + SO_4^-$ *$(+O_2) \rightarrow SO_4^{2-} + + H^+ + HO_2 + HCHO$* $\rightarrow SO_4^{2-} + H^+ + CH_2OH$	$9.0 \cdot 10^6$	2190	Clifton and Huie, 1989	"
*	152	91	$CH_3OH + NO_3$ *$(+O_2) \rightarrow NO_3^{2-} + HO_2 + HCHO$* $\rightarrow NO_3^- + H^+ + CH_2OH$	$5.4 \cdot 10^5$	4300	Herrmann and Zellner, 1998 *Exner et al., 1993*	"
*	153	92	$CH_3OH + Cl_2^-$ *$(+O_2) \rightarrow 2\ Cl^- + HO_2 + HCHO$* $\rightarrow 2\ Cl^- + H^+ + CH_2OH$	*1000* $5.1 \cdot 10^4$	5500	Zellner *et al.*, 1996	"
*	154	93	$CH_3OH + Br_2^-$ *$(+O_2) \rightarrow 2\ Br^- + HO_2 + HCHO$* $\rightarrow 2\ Br^- + H^+ + CH_2OH$	*$5.4 \cdot 10^5$* 1000		*Wicktor, 1997* Reese, 1997	"
*	155	94	$CH_3OH + CO_3^-$ *$(+O_2) \rightarrow CO_3^{2--} + HO_2 + HCHO$* **$\rightarrow CO_3^{2-} + H^+ + CH_2OH$**	$2.6 \cdot 10^3$		Zellner *et al.*, 1996	"
	156		$CH_2OH + O_2 \rightarrow O_2CH_2OH$	$2 \cdot 10^9$		von Sonntag, 1987	explicite consideration of alkyl /peroxyl radicals
*	157		$O_2CH_2OH + OH^- \rightarrow HCHO + H_2O + O_2^-$	$1.65 \cdot 10^{10}$		von Sonntag, 1987	"
	158		$O_2CH_2OH + O_2CH_2OH \rightarrow CH_3OH + O_2 + HCHO$	$1.05 \cdot 10^9$		von Sonntag, 1987	"
	159	95	$EtOH + OH$ *$(+O_2) \rightarrow H_2O + HO_2 + CH_3CHO$* $\rightarrow H_2O + CH_3CHOH$	$1.9 \cdot 10^9$		Buxton *et al.*, 1988a	split into elementary steps
*	160	96	$EtOH + SO_4^-$ *$(+O_2) \rightarrow SO_4^{2-} + + H^+ + HO_2 + CH_3CHO$* $\rightarrow SO_4^{2-} + H^+ + CH_3CHOH$	$4.1 \cdot 10^7$	1760	Clifton and Huie, 1989	"
*	161	97	$EtOH + NO_3$ *$(+O_2) \rightarrow NO_3^{2-} + HO_2 + CH_3CHO$* $\rightarrow NO_3^- + H^+ + CH_3CHOH$	$2.2 \cdot 10^6$	3300	Herrmann and Zellner, 1998	"
*	162	98	$EtOH + Cl_2^-$ *$(+O_2) \rightarrow 2\ Cl^- + HO_2 + CH_3CHO$* $\rightarrow 2\ Cl^- + H^+ + CH_3CHOH$	$1.2 \cdot 10^5$		Zellner *et al.*, 1996	"
*	163	99	$EtOH + Br_2^-$ *$(+O_2) \rightarrow 2\ Br^- + HO_2 + CH_3CHO$* $\rightarrow 2\ Br^- + H^+ + CH_3CHOH$	$3.8 \cdot 10^3$		Reese *et al.*, 1999	"
*	164	100	$EtOH + CO_3^-$ *$(+O_2) \rightarrow CO_3^{2-} + HO_2 + CH_3CHO$* $\rightarrow CO_3^{2-} + H^+ + CH_3CHOH$	$1.5 \cdot 10^4$		Khuz'min, 1972	"
	165		$CH_3CHOH + O_2 \rightarrow O_2CH_3CHOH$	$2 \cdot 10^9$		estimated	explicite consideration of alkyl /peroxyl radicals
	166		$O_2CH_3CHOH \rightarrow CH_3CHO + HO_2$	52	7217	von Sonntag, 1987	"
*	167		$O_2CH_3CHOH + OH^- \rightarrow CH_3CHO + H_2O + O_2^-$	$8 \cdot 10^9$		von Sonntag, 1987	"

	168	101	$CH_2(OH)_2 + OH$ *(+O_2) → $H_2O + HO_2 + HCOOH$* → $H_2O + CH(OH)_2$	$1.0 \cdot 10^9$	1020	Hart *et al.*, 1964; Chin and Wine, 1994	split into elementary steps
*	169	102	$CH_2(OH)_2 + SO_4^-$ *(+O_2) → $SO_4^{2-} + H^+ + HO_2 +$ HCOOH* → $SO_4^{2-} + H^+ + CH(OH)_2$	$1.4 \cdot 10^7$	1300	Buxton *et al.*, 1990	"
*	170	103	$CH_2(OH)_2 + NO_3$ *(+O_2) → $NO_3^- + HO_2 + HCOOH$* → $NO_3^- + H^+ + CH(OH)_2$	$1.0 \cdot 10^6$	4500	Exner *et al.*, 1993	"
*	171	104	$CH_2(OH)_2 + Cl_2^-$ *(+O_2) → $2\ Cl^- + HO_2 + HCOOH$* → $2\ Cl^- + H^+ + CH(OH)_2$	*$3.1 \cdot 10^4$* $3.6 \cdot 10^4$	*4400* 4330	*Zellner et al., 1996* Jacobi *et al.*, 1999	" more actual data
*	172	105	$CH_2(OH)_2 + Br_2^-$ *(+O_2) → $2\ Br^{--} + HO_2 + HCOOH$* → $2\ Br^- + H^+ + CH(OH)_2$	$3 \cdot 10^3$		estimated	split into elementary steps
*	173	106	$CH_2(OH)_2 + CO_3^-$ *(+O_2) → $CO_3^{2-} + HO_2 + HCOOH$* → $CO_3^{2-} + H^+ + CH(OH)_2$	$1.3 \cdot 10^4$		Zellner *et al.*, 1996	"
	174		$CH(OH)_2 + O_2 \rightarrow HO_2 + HCOOH$	$2 \cdot 10^9$		estimated	explicite consideration of alkyl /peroxyl radicals
	175	107	$CH_3CH(OH)_2 + OH$ *(+O_2) → $H_2O + HO_2 +$ HAc* → $H_2O + CH_3C(OH)_2$	$1.2 \cdot 10^9$		Schuchmann and von Sonntag, 1988	split into elementary steps
	176	108	$CH_3CHO + OH$ *(+$H_2O + O_2$) → $H_2O + HO_2 +$ HAc* → $H_2O + CH_3C(OH)_2$	$3.6 \cdot 10^9$		Schuchmann and von Sonntag, 1988	"
*	177	109	$CH_3CHO + SO_4^-$ *(+$H_2O + O_2$) → $SO_4^{2-} + H^+ + HO_2 +$ HAc* → $SO_4^{2-} + H^+ + CH_3CO$	$2 \cdot 10^7$		estimated	"
*	178	110	$CH_3CH(OH)_2 + SO_4^-$ *(+ O_2) → $SO_4^{2-} + H^+ + HO_2 +$ HAc* → $SO_4^{2-} + H^+ + CH_3C(OH)_2$	$2 \cdot 10^7$		estimated	"
*	179	111	$CH_3CH(OH)_2 + NO_3$*(+ O_2)→ $NO_3^- + H^+ + HO_2 +$ HAc* → $NO_3^- + H^+ + CH_3C(OH)_2$	$1.9 \cdot 10^6$		Zellner *et al.*, 1996	"
*	180	112	$CH_3CHO + Cl_2^-$ *(+ O_2) → $2\ Cl^- + H^+ + HO_2 +$ HAc* → $2\ Cl^- + H^+ + CH_3CO$	$4 \cdot 10^4$		Jacobi, 1996	"
*	181	113	$CH_3CHO + Br_2^-$ *(+ O_2) → $2\ Br^- + H^+ + HO_2 +$ HAc* → $2\ Br^- + H^+ + CH_3CO$	*$4 \cdot 10^4$* **$4 \cdot 10^3$**		*estimated* estimated: $k_{Br2-} = 0.1 \cdot k_{Cl2-}$	" better estimate
*	182	114	$CH_3CHO + CO_3^-$ *(+ O_2) → $CO_3^{2}- + H^+ + HO_2 +$ HAc* → $CO_3^{2-} + H^+ + CH_3CO$	$1 \cdot 10^4$		estimated	split into elementary steps
	183	115	$HCOOH + OH$ *(+ O_2) → $H_2O + HO_2 + CO_2$* → $H_2O + CO_2H$	$1.3 \cdot 10^8$	1000	Buxton *et al.*, 1988a; Chin and Wine, 1994	"
	184	116	$HCOO^- + OH$ *(+ O_2) → $OH^- + HO_2 + CO_2$* → $OH^- + CO_2H$	*$\cdot 10^9$* **$3.2 \cdot 10^9$**	1000	Buxton *et al.*, 1988a; Elliot and Simsons, 1984	"

*	185	117	$HCOOH + SO_4^- \mathit{(+ O_2)} \rightarrow \mathit{SO_4^{2-} + H^+ + HO_2 + CO_2}$ $\rightarrow SO_4^{2-} + H^+ + CO_2H$	$2.5 \cdot 10^6$		Reese, 1997	"
*	186	118	$HCOO^- + SO_4^- \mathit{(+ O_2)} \rightarrow \mathit{SO_4^{2-} + HO_2 + CO_2}$ $\rightarrow SO_4^{2-} + CO_2H$	$2.1 \cdot 10^7$		Reese, 1997	"
*	187	119	$HCOOH + NO_3 \mathit{(+ O_2)} \rightarrow \mathit{NO_3^- + H^+ + HO_2 + CO_2}$ $\rightarrow \mathbf{NO_3^- + H^+} + CO_2H$	$3.8 \cdot 10^5$	3400	Exner *et al.*, 1994	"
*	188	120	$HCOO^- + NO_3 \mathit{(+ O_2)} \rightarrow \mathit{NO_3^- + HO_2 + CO_2}$ $\rightarrow \mathbf{NO_3^-} + CO_2H$	$5.1 \cdot 10^7$	2200	Exner *et al.*, 1994	"
*	189	121	$HCOOH + Cl_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Cl^- + H^+ + HO_2 + CO_2}$ $\rightarrow 2\,Cl^- + H^+ + CO_2H$	*5500* $8 \cdot 10^4$	*4500* 4450	*Jacobi et al., 1999* Jacobi *et al.*, 1999	" more actual value
*	190	122	$HCOO^- + Cl_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Cl^- + HO_2 + CO_2}$ $\rightarrow 2\,Cl^- + CO_2H$	$1.3 \cdot 10^6$		*Jacobi et al., 1996* Jacobi *et al.*, 1999	split into elementary steps
*	191	123	$HCOOH + Br_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Br^- + H^+ + HO_2 + CO_2}$ $\rightarrow 2\,\mathbf{Br^-} + H^+ + CO_2H$	$4 \cdot 10^3$		Reese *et al.*, 1999	"
*	192	124	$HCOO^- + Br_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Br^- + HO_2 + CO_2}$ $\rightarrow 2\,\mathbf{Br^-} + CO_2H$	$4.9 \cdot 10^3$		Jacobi, 1996	"
*	193	125	$HCOO^- + CO_3^- \mathit{(+ O_2)} \rightarrow \mathit{CO_3^{2-} + H^+ + HO_2 + CO_2}$ $\rightarrow \mathbf{CO_3^{2-} + H^+ + CO_2H}$	$1.4 \cdot 10^5$	3300	Zellner *et al.*, 1996	"
	194	126	$CO_2H + O_2 \rightarrow CO_2 + HO_2$	$2 \cdot 10^9$		estimated	explicite consideration of alkyl /peroxyl radicals
	195	127	$HAc + OH \mathit{(+ O_2)} \rightarrow \mathit{H_2O + HO_2 + ACO_3}$ $\rightarrow H_2O + CH_2COOH$	$1.5 \cdot 10^7$	1330	Thomas, 1965; Chin and Wine, 1994	split into elementary steps
	196	128	$Ac^- + OH \mathit{(+ O_2)} \rightarrow \mathit{OH^- + HO_2 + ACO_3}$ $\rightarrow H_2O + CH_2COO^-$	$1 \cdot 10^8$	1800	Fisher and Hamill, 1973; Chin and Wine, 1994	"
*	197	129	$HAc + SO_4^- \mathit{(+ O_2)} \rightarrow \mathit{SO_4^{2-} + H^+ + HO_2 + ACO_3}$ $\rightarrow \mathbf{SO_4^{2-} + H^+} + CH_2COOH$	$2.0 \cdot 10^5$		Reese, 1997	"
*	198	130	$Ac^- + SO_4^- \mathit{(+ O_2)} \rightarrow \mathit{SO_4^{2-} + CH_3O_2 + CO_2}$ $\rightarrow \mathbf{SO_4^{2-} + CH_3 + CO_2}$	$2.8 \cdot 10^7$	1210	Reese, 1997; Huie and Clifton, 1990	"
*	199	131	$HAc + NO_3 \mathit{(+ O_2)} \rightarrow \mathit{NO_3^- + H^+ + HO_2 + ACO_3}$ $\rightarrow \mathbf{NO_3^- + H^+} + CH_2COOH$	$1.4 \cdot 10^4$	3800	Exner *et al.*, 1994	"
*	200	132	$Ac^- + NO_3 \mathit{(+ O_2)} \rightarrow \mathit{NO_3^- + CH_3O_2 + CO_2}$ $\rightarrow \mathbf{NO_3^- + CH_3 + CO_2}$	$2.9 \cdot 10^6$	3800	Exner *et al.*, 1994	"
*	201	133	$HAc + Cl_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Cl^- + H^+ + HO_2 + ACO_3}$ $\rightarrow \mathbf{2\,Cl^- + H^+} + CH_2COOH$	*1950* 1500	*4800* 4930	*Jacobi et al., 1998* Jacobi *et al.*, 1999	" more actual value
*	202	134	$Ac^- + Cl_2^- \mathit{(+ O_2)} \rightarrow \mathit{2\,Cl^- + CH_3O_2 + CO_2}$ $\rightarrow \mathbf{2\,Cl^- + CH_3 + CO_2}$	$2.6 \cdot 10^5$	4800	Jacobi *et al.*, 1996	split into elementary steps

*	203	135	$HAc + Br_2^- (+ O_2) \rightarrow 2 Br^- + H^+ + HO_2 + ACO_3$ $\rightarrow$ **$2 Br^- + H^+$** $+ CH_2COOH$	10		Reese *et al.*, 1999	"
*	204	136	$Ac^- + Br_2^- (+ O_2) \rightarrow 2Br^- + CH_3O_2 + CO_2$ **$\rightarrow 2 Br^- + CH_3 + CO_2$**	100		Jacobi, 1996	"
*	205	137	$Ac^- + CO_3^- (+ O_2) \rightarrow CO_3^{2-} + CH_3O_2 + CO_2$ **$\rightarrow CO_3^{2-} + CH_3 + CO_2$**	580		Zellner *et al.*, 1996	"
	206		$CH_2COOH + O_2 \rightarrow ACO_3$	$1.7 \cdot 10^9$		Schuchmann *et al.*, 1985	explicite consideration of alkyl /peroxyl radicals
	207		$CH_3 + O_2 \rightarrow CH_3O_2$	$4.1 \cdot 10^9$		Marchaj *et al.*, 1991	"
	208	138	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	$1.7 \cdot 10^8$	2200	Herrmann *et al.*, 1999b)	
	209		$CH_3O_2 + CH_3O_2 \rightarrow CH_3O + CH_3O + O_2$	$3.6 \cdot 10^7$	2200	Herrmann *et al.*, 1999b)	consideration of additional reaction pathways (correlation)
	210		$ACO_3 + ACO_3 \rightarrow 2 CH_3O_2 + 2 CO_2 + O_2$	$1.5 \cdot 10^8$		estimated equal as $k_{(2\ ETHPX)}$	correct products;
	211	139	$CH_3O_2 + HSO_3^- \rightarrow CH_3OOH + SO_3^-$	$5 \cdot 10^5$		Herrmann *et al.*, 1999b)	
*	212	140	$ETHP + ETHP \rightarrow$ *products* $\rightarrow EtOH + CH_3CHO + O_2$	*$1.6 \cdot 10^8$* $6 \cdot 10^7$	-750	Herrmann *et al.*, 1999	correct products; consideration of different reaction pathways (correlation)
	213		$ETHP + ETHP \rightarrow CH_3CH_2O + CH_3CH_2O + O_2$	$1 \cdot 10^8$	-750	Herrmann *et al.*, 1999	correct products; consideration of different reaction pathways (correlation)
*	214		$CH_3CH_2O + O_2 \rightarrow HO_2 + CH_3CHO$	$6 \cdot 10^6$		estimated	sink reaction
	215		$CH_3CH_2O \rightarrow CH_3CHOH$	$1 \cdot 10^6$		estimated	sink reaction
*	216		$Fe^{2+} + CH_3O_2 \rightarrow FeCH_3O_2^{2+}$	$8.6 \cdot 10^5$		Khaikin *et al.*, 1996	$FeCH_3O_2^+$: new considered
*	217		$FeCH_3O_2^{2+} + H^+ \rightarrow Fe^{3+} + O_2$	$3.0 \cdot 10^4$		Khaikin *et al.*, 1996	$FeCH_3O_2^+$: new considered
*	218		$FeCH_3O_2^{2+} \rightarrow Fe^{3+} + CH_3OOH + OH^-$	100		Khaikin *et al.*, 1996	$FeCH_3O_2^+$: new considered
	219		$OH + HC_2O_4^- \rightarrow H_2O + C_2O_4^-$	$3.2 \cdot 10^7$		Getoff *et al.*, 1971	consideration of C_2-difunctional compounds
*	220		$NO_3 + HC_2O_4^- \rightarrow NO_3^- + H^+ + C_2O_4^-$	$6.8 \cdot 10^7$		Raabe, 1996	"
*	221		$Cl_2^- + HC_2O_4^- \rightarrow 2 Cl^- + H^+ + C_2O_4^-$	$1.3 \cdot 10^6$		estimated (ETR)	"
*	222		$Br_2^- + HC_2O_4^- \rightarrow 2 Br- + H^+ + C_2O_4^-$	$3.7 \cdot 10^3$		estimated (ETR)	"
*	223		$SO_4^- + HC_2O_4^- \rightarrow SO_4^{2-} + H^+ + C_2O_4^-$	$3.35 \cdot 10^5$		Buxton *et al.*, 1999	"
	224		$OH + C_2O_4^{2-} \rightarrow OH^- + C_2O_4^-$	$5.3 \cdot 10^6$		Getoff *et al.*, 1971	"
*	225		$NO_3 + C_2O_4^{2-} \rightarrow NO_3^- + C_2O_4^-$	$2.2 \cdot 10^8$		Raabe, 1996	"
*	226		$Cl_2^- + C_2O_4^{2-} \rightarrow 2 Cl^- + H^+ + C_2O_4^-$	$4.0 \cdot 10^6$		estimated (ETR)	"
*	227		$Br_2^- + C_2O_4^{2-} \rightarrow 2 Br- + C_2O_4^-$	$1.1 \cdot 10^4$		estimated (ETR)	"
*	228		$SO_4^- + C_2O_4^{2-} \rightarrow SO_4^{2-} + C_2O_4^-$	$1.05 \cdot 10^6$		Buxton *et al.*, 1999a	"
	229		$C_2O_4^- + O_2 \rightarrow CO_2 + CO_2 + O_2^-$	$2.0 \cdot 10^9$		estimated	"
	230		$OH + CH(OH)_2CH(OH)_2 \rightarrow H_2O + C(OH)_2CH(OH)_2$	$1.1 \cdot 10^9$	1516	Buxton *et al.*, 1997	"

*	231		$NO_3 + CH(OH)_2CH(OH)_2 \rightarrow H^+ + NO_3^- + C(OH)_2CH(OH)_2$	$1.1 \cdot 10^6$	3368	Herrmann *et al.*, 1995c	"
*	232		$Cl_2^- + CH(OH)_2CH(OH)_2 \rightarrow H^+ + 2\ Cl^- + C(OH)_2CH(OH)_2$	$4.0 \cdot 10^4$		Herrmann *et al.*, 1995c	"
*	233		$Br_2^- + CH(OH)_2CH(OH)_2 \rightarrow H^+ + 2\ Br^- + C(OH)_2CH(OH)_2$	500		estimated (H abstr.)	"
*	234		$SO_4^- + CH(OH)_2CH(OH)_2 \rightarrow H^+ + SO_4^{2-} + C(OH)_2CH(OH)_2$	$2.35 \cdot 10^7$	1395	Mirabel *et al.*, 1996	"
	235		$C(OH)_2CH(OH)_2 + O_2 \rightarrow O_2C(OH)_2CH(OH)_2$	$1.38 \cdot 10^9$		Mirabel *et al.*, 1996	"
	236		$O_2C(OH)_2CH(OH)_2 \rightarrow HO_2 + CH(OH)_2COOH$	$2 \cdot 10^9$		estimated	"
	237		$OH + CH(OH)_2COOH \rightarrow H_2O + C(OH)_2COOH$	$1.1 \cdot 10^9$	1516	estimate equal as k ((CH(OH)$_2$)	"
*	238		$NO_3 + CH(OH)_2COOH \rightarrow H^+ + NO_3^- + C(OH)_2COOH$	$1.1 \cdot 10^6$	3368	estimate equal as k ((CH(OH)$_2$)	"
*	239		$Cl_2^- + CH(OH)_2COOH \rightarrow H^+ + 2\ Cl^- + C(OH)_2COOH$	$4.0 \cdot 10^4$		estimate equal as k ((CH(OH)$_2$)	"
*	240		$Br_2^- + CH(OH)_2COOH \rightarrow H^+ + 2\ Br^- + C(OH)_2COOH$	500		estimate equal as k ((CH(OH)$_2$)	"
*	241		$SO_4^- + CH(OH)_2COOH \rightarrow H^+ + SO_4^{2-} + C(OH)_2COOH$	$2.35 \cdot 10^7$	1395	estimate equal as k ((CH(OH)$_2$)	"
	242		$C(OH)_2COOH + O_2 \rightarrow O_2C(OH)_2COOH$	$2 \cdot 10^9$		estimated	additional reactions of peroxyl radicals
	243		$O_2C(OH)_2COOH \rightarrow HO_2 + H_2C_2O_4$	$2 \cdot 10^9$		estimated	"
*	244		$CH_3CO + O_2 \rightarrow ACO_3$	$2 \cdot 10^9$		estimated	"
*	245		$ACO_3 + O_2^- \rightarrow CH_3C(O)OO^-$	$1 \cdot 10^9$		Schuchmann and v. Sonntag, 1988	"
	246		$CH_3C(OH)_2 + O_2 \rightarrow CH_3C(OH)_2O_2$	$2 \cdot 10^9$		estimated	"
	247		$CH_3C(OH)_2O_2 \rightarrow 2\ H^+ + Ac^- + O_2^-$	$1 \cdot 10^5$		estimated	"
*	248		$CH_3O + O_2 \rightarrow HCHO + HO_2$	$1.2 \cdot 10^6$		estimated as in the gas phase	"
	249		$CH_3O \rightarrow CH_2OH$	$1 \cdot 10^6$		estimated	"
	250		$2\ O_2CH_2COO^- (+ H_2O) \rightarrow 2\ CH(OH)_2COO^- + H_2O_2$	$2 \cdot 10^7$		Schuchmann *et al.*, 1985	"
*	251		$2\ O_2CH_2COO^- \rightarrow 2\ HCHO + H_2O_2 + 2\ OH^- + 2\ CO_2$	$1.88 \cdot 10^7$		Schuchmann *et al.*, 1985	"
*	252		$2\ O_2CH_2COO^- (+ H_2O) \rightarrow CH(OH)_2COO^- + CH_3COO^- + O_2$	$1.88 \cdot 10^7$		Schuchmann *et al.*, 1985	"
*	253		$2\ O_2CH_2COO^- (+ H_2O) \rightarrow 2\ O_2^- + CH(OH)_2COO^- + 2\ H_2O$	$7.5 \cdot 10^6$		Schuchmann *et al.*, 1985	"
	254		$CO_2^- + O_2 \rightarrow CO_2 + O_2^-$	$4 \cdot 10^9$		estimated	"
	255		$CH_2COO^- + O_2 \rightarrow O_2CH_2COO^-$	$2 \cdot 10^9$			"

Table 8: **Chlorine chemistry**

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\,s^{-1}$	E_a / R, K	Reference	comment
	256	141	*$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$—*	*$3.3 \cdot 10^8$*	*0*	*Huie and Clifton, 1990; Herrmann et al., 1997*	back reaction included => E51
	257	142	*$NO_3 + Cl^- \rightarrow NO_3^- + Cl$*	*$1.0 \cdot 10^7$*	*4300*	*Exner et al., 1992*	back reaction included => E52
*	258	143	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2\,Cl^-$	$8.7 \cdot 10^8$		Zellner *et al.*, 1996	
	259	144	$Cl_2^- + Fe^{2+} \rightarrow 2\,Cl^- + Fe^{3+}$	$1.0 \cdot 10^7$	3030	Thornton and Laurence, 1973	
*	260		$Cl_2^- + Fe^{2+} \rightarrow FeCl^{2+}$	$4 \cdot 10^6$	3490	Thornton and Laurence, 1973	additional ramification
*	261	145	$Cl_2^- + Mn^{2+} \rightarrow 2\,Cl^- + Mn^{3+}$	$8.5 \cdot 10^6$	4090	Laurence and Thornton, 1973	
*	262		$Cl_2^- + Mn^{2+} \rightarrow MnCl_2^+$	$2 \cdot 10^7$	4090	Laurence and Thornton, 1973	additional ramification
*	263		$MnCl_2^+ \rightarrow Mn^{2+} + Cl_2^-$	$3 \cdot 10^5$		Laurence and Thornton, 1973	following sinks
*	264		$MnCl_2^+ \rightarrow Mn^{3+} + 2\,Cl^-$	$2.1 \cdot 10^5$		Laurence and Thornton, 1973	"
*	265	146	$Cl_2^- + Cu^+ \rightarrow 2\,Cl^- + Cu^{2+}$	*$1 \cdot 10^7$* $1 \cdot 10^8$		*$k_{Cu+} = k_{Fe2+}$* $k_{Cu+} \cong 10 \cdot k_{Fe2+}$	better estimate (more consistent to other Cl_2^-/Br_2^- ratios)
*	266	147	$Cl_2^- + H_2O_2 \rightarrow 2\,Cl^- + H^+ + HO_2$	*$7 \cdot 10^5$* **$5 \cdot 10^4$**	3340	*Elliot, 1989* **Jacobi *et al.*, 1999**	more actual value
*	267	148	$Cl_2^- + CH_3OOH \rightarrow 2\,Cl^- + H^+ + CH_3O_2$	*$7 \cdot 10^5$* $5 \cdot 10^4$	3340	$k_{CH3OOH} = k_{H2O2}$	
*	268	149	$Cl_2^- + OH^- \rightarrow 2\,Cl^- + OH$	$4.0 \cdot 10^6$		Jacobi, 1996	
	269	150	$Cl_2^- + HO_2 \rightarrow 2\,Cl^- + H^+ + O_2$	$1.3 \cdot 10^{10}$		Jacobi, 1996	
*		151	$Cl_2^- + O_2^- \rightarrow 2\,Cl^- + O_2$	$6 \cdot 10^9$		Jacobi, 1996	
	270	152	$Cl_2^- + HSO_3^- \rightarrow 2\,Cl^- + H^+ + SO_3^-$	$1.7 \cdot 10^8$	400	Jacobi *et al.*, 1996	
*	271	153	$Cl_2^- + SO_3^{2-} \rightarrow 2\,Cl^- + SO_3^-$	$6.2 \cdot 10^7$		Jacobi *et al.*, 1996	
	272	154	$Cl_2 + H_2O \rightarrow H^+ + Cl^- + HOCl$	*0.401* **0.4**	7900	Wang and Margerum, 1994	correct rounded
	273		**$Cl_2^- + H_2O \rightarrow H^+ + 2\,Cl^- + OH$**	**6**		**Jacobi, 1996**	new data available

Table 9: Bromine chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Reference	comment
	274	155	$SO_4^- + Br^- \rightarrow SO_4^{2-} + Br$	$2.1 \cdot 10^9$		Herrmann *et al.*, 1997	
	275	156	$NO_3 + Br^- \rightarrow NO_3^- + Br$	$3.8 \cdot 10^9$		Zellner *et al.*, 1996	
	276	157	$Br_2^- + Br_2^- \rightarrow Br_2 + 2\ Br^-$	$1.7 \cdot 10^9$		*Reese, 1998* Reese *et al.*, 1999	better reference
	277	158	$Br_2^- + Fe^{2+} \rightarrow 2\ Br^- + Fe^{3+}$	$3.6 \cdot 10^6$	3330	Thornton and Laurence, 1973	
*	278		$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.3 \cdot 10^6$	4330	Laurence and Thornton, 1973	additional ramification
*	279	159	$Br_2^- + Mn^{2+} \rightarrow 2\ Br^- + Mn^{3+}$	$6.3 \cdot 10^6$	4330	Laurence and Thornton, 1973	
*	280		$MnBr_2^+ \rightarrow Br_2^- + Mn^{2+}$	$3 \cdot 10^5$		Laurence and Thornton, 1973	additional ramification
*	281		$MnBr_2^+ \rightarrow 2\ Br^- + Mn^{3+}$	$2.2 \cdot 10^5$		Laurence and Thornton, 1973	following sink
	282	160	$Br_2^- + Cu^+ \rightarrow 2\ Br^- + Cu^{2+}$	$3.6 \cdot 10^6$		$k_{Cu+} = k_{Fe2+}$	
	283	161	$Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$	$1.0 \cdot 10^5$		Reese, 1997	
*	284	162	$Br_2^- + MHP \rightarrow 2\ Br^- + H^+ + CH_3O_2$	$1.0 \cdot 10^5$		$k_{R174} = k_{R172}$	
*	285	163	$Br_2^- + OH^- \rightarrow 2\ Br^- + OH$	$1.1 \cdot 10^4$		Jacobi, 1996	
	286	164	$Br_2^- + HO_2 \rightarrow 2\ Br^- + H^+ + O_2$	$6.5 \cdot 10^9$		Rafi and Sutton, 1965	
*	287	165	$Br_2^- + O_2^- \rightarrow 2\ Br^- + O_2$	$1.7 \cdot 10^8$		Wagner and Strehlow, 1987	
	288	166	$Br_2^- + HSO_3^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	$5.0 \cdot 10^7$	780	Shoute *et al.*, 1991; Jacobi, 1996	
*	289	167	$Br_2^- + SO_3^{2-} \rightarrow 2\ Br^- + SO_3^-$	$3.3 \cdot 10^7$	650	Shoute *et al.*, 1991; Jacobi, 1996	
	290	168	$Br_2 + H_2O \rightarrow Br^- + H^+ + HOBr$	1.7	7500	Beckwith *et al.*, 1996	
	291		$BrOH^- \rightarrow Br + OH^-$	$4.2 \cdot 10^6$		Zehavi and Rabani, 1972	completion of $BrOH^-$ chemistry

<u>Table 10:</u> Carbonate Chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Reference	comment
*	292	169	$HCO_3^- + OH \rightarrow H_2O + CO_3^-$	$1.7 \cdot 10^7$	1900	Exner, 1990	
*	293	170	$CO_3^{2-} + OH \rightarrow OH^- + CO_3^-$	$3.9 \cdot 10^8$	2840	Buxton *et al.*, 1988a,**b**	
*	294	171	$CO_3^{2-} + SO_4^- \rightarrow SO_4^{2-} + CO_3^-$	*4.1 · 10^7*		*estimated*	measurement instead of estimate
				$4.1 \cdot 10^6$		Padmaja *et al.*, 1993	
*	295	172	$HCO_3^- + SO_4^- \rightarrow SO_4^{2-} + CO_3^- + H^+$	$2.8 \cdot 10^6$	2090	Huie and Clifton, 1990	
*	296	173	$CO_3^{2-} + NO_3 \rightarrow NO_3^- + CO_3^-$	$4.1 \cdot 10^7$		estimated	
*	297		$HCO_3^- + NO_3 \rightarrow NO_3^- + CO_3^- + H^+$	$4.1 \cdot 10^7$		estimated $k_{HCO3-} = k_{CO32-}$	reactions of HCO_3^- added for completion
*	298	174	$CO_3^{2-} + Cl_2^- \rightarrow 2\ Cl^- + CO_3^-$	$2.7 \cdot 10^6$		estimated	
*	299		$HCO_3^- + Cl_2^- \rightarrow 2\ Cl^- + CO_3^- + H^+$	$2.7 \cdot 10^6$		estimated	reactions of HCO_3^- added for completion
*	300	175	$CO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + CO_3^-$	$1.1 \cdot 10^5$		Huie *et al.*, 1991b	
*	301		$HCO_3^- + Br_2^- \rightarrow 2\ Cl^- + CO_3^-$	$1.1 \cdot 10^5$		estimated	reactions of HCO_3^- added for completion
*	302	176	$CO_3^- + CO_3^-\ (+ O_2) \rightarrow\ 2\ O_2^- + 2\ CO_2$	$2.2 \cdot 10^6$		Huie and Clifton, 1990	
*	303	177	$CO_3^- + Fe^{2+} \rightarrow CO_3^{2-} + Fe^{3+}$	$2 \cdot 10^7$		estimated	
*	304	178	$CO_3^- + Mn^{2+} \rightarrow CO_3^{2-} + Mn^{3+}$	$1.5 \cdot 10^7$		Cope *et al.*, 1978	
*	305	179	$CO_3^- + Cu^+ \rightarrow CO_3^{2-} + Cu^{2+}$	$2 \cdot 10^7$		estimated	
*	306	180	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	$4.3 \cdot 10^5$		Draganic *et al.*, 1991	
*	307	181	$CO_3^- + CH_3OOH \rightarrow HCO_3^- + CH_3O_2$	$4.3 \cdot 10^5$		$k_{H2O2} = k_{CH3OOH}$	
*	308	182	$CO_3^- + HO_2 \rightarrow HCO_3^- + O_2$	$6.5 \cdot 10^8$		$k_{HO2} = k_{O2-}$	
*	309	183	$CO_3^- + O_2^- \rightarrow CO_3^{2-} + O_2$	$6.5 \cdot 10^8$		Eriksen *et al.*, 1985	
*	310	184	$CO_3^- + HSO_3^- \rightarrow HCO_3^- + SO_3^-$	$1 \cdot 10^7$		estimated	
*	311	185	$CO_3^- + SO_3^{2-} \rightarrow CO_3^{2-} + SO_3^-$	$5.0 \cdot 10^6$	470	Exner *et al.*, 1990; Huie *et al.*, 1991a	
*	312		$CO_3^- + NO_2 \rightarrow CO_2 + NO_3^-$	$1 \cdot 10^9$		Lilie *et al.*, 1978	sinks added for CO_3^-
*	313		$CO_3^- + O_3 \rightarrow CO_2 + O_2 + O_2^-$	$1 \cdot 10^5$		Sehested *et al.*, 1983	sinks added for CO_3^-

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

red.	No 2.4	No 2.3	Reaction	j_{max} [s^{-1}]	Range of Quantum Yield Φ	References	comment
	314	186	$H_2O_2 + h\nu \rightarrow 2\ OH$	$7.19 \cdot 10^{-6}$	0.98 ± 0.03^a 0.96 ± 0.03^b	Zellner *et al.*, 1990 Zellner *et al.*, 1990	
	315	187	$[Fe(OH)]^{2+} + h\nu \rightarrow Fe^{2+} + OH$	$4.51 \cdot 10^{-3}$	0.312 ± 0.03 ... 0.074 ± 0.015^c	Benkelberg and Warneck, 1995	
*	316	188	$[Fe(OH)_2]^+ + h\nu \rightarrow Fe^{2+} + OH + OH^-$	$5.77 \cdot 10^{-3}$	$0.255....0.07^d$	Benkelberg *et al.*, 1991	
*	317	189	$[Fe(SO_4)]^+ + h\nu \rightarrow Fe^{2+} + SO_4^-$	$6.43 \cdot 10^{-3}$	$(7.9 \pm 0.34....1.56 \pm 0.02) \cdot 10^{-3\ c}$	Benkelberg and Warneck,1995	
*	318	190	$NO_2^- + h\nu\ (+ H^+) \rightarrow NO + OH$	$2.57 \cdot 10^{-5}$	0.07 ± 0.01^a 0.046 ± 0.009^b	Zellner *et al.*, 1990 Zellner *et al.*, 1990	
	319	191	$NO_3^- + h\nu\ (+ H^+) \rightarrow NO_2 + OH$	$4.28 \cdot 10^{-7}$	0.017 ± 0.003	Zellner *et al.*, 1990	
	320		$[Fe(C_2O_4)_2]^- + h\nu \rightarrow Fe^{2+} + C_2O_4^{2-} + C_2O_4^-$	$2.47 \cdot 10^{-2}$	1.0 ± 0.25 (436 nm)	Zuo and Hoigné, 1992	oxalate chemistry
*	321		$[Fe(C_2O_4)_3]^{3-} + h\nu \rightarrow Fe^{2+} + 2\ C_2O_4^{2-} + C_2O_4^-$	$1.55 \cdot 10^{-2}$	0.6 ± 0.46 (436 nm)	Zuo and Hoigné, 1992	"
*	322		$CH_3O_2H + h\nu \rightarrow CH_3O + OH$	$7.19 \cdot 10^{-6}$		$j_{P1} = j_{P9}$	analogous to H_2O_2 (also other reactions treated as being equal)
*	323		$NO_3 + h\nu \rightarrow NO + O_2$	$2.32 \cdot 10^{-2}$		estimated as in the gas phase	additional sinks for NO_3
*	324		$NO_3 + h\nu \rightarrow NO_2 + O^3P$	$2.01 \cdot 10^{-1}$		estimated as in the gas phase	additional sinks for NO_3

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

Table 12: Aqueous phase equilibria

red.	No 2.4	No 2.3	Reactions	K, M	k_{298}, (forward) $M^{-n}\ s^{-1}$	E_a / R, K	Ref.	k_{298} (back) $M^{-n}\ s^{-1}$	E_a / R, K	Ref.	comment
	1	1	$H_2O \rightleftharpoons H^+ + OH^-$	$1.8 \cdot 10^{-16}$	$2.34 \cdot 10^{-5}$	6800	a	$1.3 \cdot 10^{11}$		c	
	2	2	$CO_2 + H_2O \rightleftharpoons H_2CO_3$	$7.7 \cdot 10^{-7}$	$4.3 \cdot 10^{-2}$	9250	b	$5.6 \cdot 10^4$	8500	x	
	3	3	$H_2CO_3 \rightleftharpoons H^+ + HCO_3^-$	$2 \cdot 10^{-4}$	$1 \cdot 10^7$		c	$5 \cdot 10^{10}$		c	
*	4	4	$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$	$4.69 \cdot 10^{-11}$	2.35	1820	a	$5 \cdot 10^{10}$		c	
	5	5	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72 \cdot 10^6$	*$8.6 \cdot 10^{16}$* $5 \cdot 10^{11}$	-6890	d	*$5 \cdot 10^{10}$* $2.9 \cdot 10^5$		c	$8.6 \cdot 10^{16}$ >> diffusion controlled (vibrational freq.); based on K $\cdot k_{back}$ new: k_f = speed of hydrogen bond breaking in water
	6	6	$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-$	| *$1.77 \cdot 10^{-5}$* $3.17 \cdot 10^{-7}$	| $6.02 \cdot 10^5$	560	a	$3.4 \cdot 10^{10}$		c	H_2O included in K
	7	7	$HO_2 \rightleftharpoons H^+ + O_2^-$	$1.6 \cdot 10^{-5}$	$8.0 \cdot 10^5$	0	e, f	$5 \cdot 10^{10}$	0	y	
	8	8	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	22	$1.1 \cdot 10^{12}$	-1800	g, h	$5 \cdot 10^{10}$		c	
	9	9	$HNO_2 \rightleftharpoons H^+ + NO_2^-$	$5.3 \cdot 10^{-4}$	$2.65 \cdot 10^7$	1760	i	$5 \cdot 10^{10}$		c	
	10	10	$HO_2NO_2 \rightleftharpoons H^+ + O_2NO_2^-$	$1 \cdot 10^{-5}$	$5 \cdot 10^5$		j	$5 \cdot 10^{10}$		y	

	11	11	$NO_2 + HO_2 \rightleftharpoons HO_2NO_2$	$2.2\cdot10^{9}$	$1.0 \cdot 10^{7}$		k	$4.6 \cdot 10^{-3}$		j	
	12	12	$SO_2 + H_2O \rightleftharpoons HSO_3^- + H^+$	$3.13\cdot10^{-4}$	$6.27 \cdot 10^{4}$	-1940	l	$2.0 \cdot 10^{8}$		c	
	13	13	$HSO_3^- \rightleftharpoons SO_3^{2-} + H^+$	$6.22\cdot10^{-8}$	3110	-1960	l	$5 \cdot 10^{10}$		c	
	14		$H_2SO_4 \rightleftharpoons HSO_4^- + H^+$	**1000**	$5 \cdot \mathbf{10^{13}}$			$5 \cdot 10^{10}$		c	added for completion
	15	14	$HSO_4^- \rightleftharpoons SO_4^{2-} + H^+$	$1.02\cdot10^{-2}$	$1.02 \cdot 10^{9}$	-2700	g	$1 \cdot 10^{11}$		c	
	16	15	$HCOOH \rightleftharpoons HCOO^- + H^+$	$1.77\cdot10^{-4}$	$8.85 \cdot 10^{6}$	-12	a	$5 \cdot 10^{10}$		c	
	17	16	$HAc \rightleftharpoons Ac^- + H^+$	$1.75\cdot10^{-5}$	$8.75 \cdot 10^{5}$	-46	a	$5 \cdot 10^{10}$		c	
	18	17	$Fe^{3+} + H_2O \rightleftharpoons [Fe(OH)]^{2+} + H^+$	$1.1\cdot10^{-4}$	$4.7 \cdot 10^{4}$		m	$4.3 \cdot 10^{8}$		m	
*	19	18	$[Fe(OH)]^{2+} + H_2O \rightleftharpoons [Fe(OH)_2]^+ + H^+$	$1.4\cdot10^{-7}$	$1.1 \cdot 10^{3}$		n	$8.0 \cdot 10^{9}$		n	
*	20	19	$Fe^{3+} + SO_4^{2-} \rightleftharpoons [Fe(SO_4)]^+$	$1.8\cdot10^{-2}$	$3.2 \cdot 10^{3}$		m	$1.8 \cdot 10^{5}$		m	
	21	20	$HCHO + H_2O \rightleftharpoons CH_2(OH)_2$	36	0.18	-4030	q	$5.1 \cdot 10^{-3}$		p	
	22	21	$CH_3CHO + H_2O \rightleftharpoons CH_3CH(OH)_2$	$2.46\cdot10^{-2}$	$1.4 \cdot 10^{-4}$	-2500	p	$5.69 \cdot 10^{-3}$		o	
	23	22	$CH_2(OH)_2 + HSO_3^- \rightleftharpoons HMS^- + H_2O$	$2\cdot10^{8}$	0.436	2990	q	$2.2\cdot10^{-9}$	**2990**	q	
	24	23	$CH_2(OH)_2 + SO_3^{2-} \rightleftharpoons HMS^- + OH^-$	33	$1.35\cdot10^{5}$	2450	q	$4.15\cdot10^{3}$	5530	q	
	25	24	$Cl + Cl^- \rightleftharpoons Cl_2^-$	*$1.9\cdot10^{5}$* $1.4\cdot10^{5}$	*$2.7\cdot10^{10}$* $8.5\cdot10^{9}$		r	*$1.4\cdot10^{5}$* $6\cdot10^{4}$		r	new data available
	26	25	$Br + Br^- \rightleftharpoons Br_2^-$	$6\cdot10^{5}$	$1.2 \cdot 10^{10}$		s	$1.9 \cdot 10^{4}$		s	
	27	26	$Cl^- + OH \rightleftharpoons ClOH^-$	0.7	$4.3\cdot10^{9}$		t	$6.1\cdot10^{9}$		t	
	28	27	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	*$1.6\cdot10^{7}$* $5.1\cdot10^{6}$	$2.1\cdot10^{10}$		t	*$1.3\cdot10^{3}$* 4100		z	new data available
*	29	28	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	$2.2\cdot10^{-4}$	$1.0\cdot10^{4}$		u	$4.5\cdot10^{7}$		u	
	30	29	$Br^- + OH \rightleftharpoons BrOH^-$	333	$1.1\cdot10^{10}$		v	$3.3\cdot10^{7}$		v	
	31	30	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.8\cdot10^{12}$	$4.4\cdot10^{10}$		v	$2.45\cdot10^{-2}$		w	
*	32	31	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	70	$1.9\cdot10^{8}$		v	$2.7\cdot10^{6}$		x	
*	33		$Mn^{3+} + H_2O \rightleftharpoons Mn(OH)^{2+} + H^+$	0.93	$1.86\cdot10^{10}$		y	$2 \cdot10^{10}$		y	detailed formulation of Mn chemistry (new data available)
*	34		$O_2^- + Mn^{2+} \rightleftharpoons MnO_2^+$	$2.3\cdot10^{4}$	$1.5\cdot10^{8}$		z	$6.5\cdot10^{3}$		z	"
*	35		$HO_2 + Mn^{2+} \rightleftharpoons MnO_2^+ + H^+$	0.17	$1.1\cdot10^{6}$		z	$6.5\cdot10^{6}$		z	"
*	36		$Mn^{3+} + Mn^{3+} \rightleftharpoons Mn^{2+} + Mn^{4+}$	$1\cdot10^{-3}$	$1\cdot10^{7}$		A	$1\cdot10^{10}$		A	"
*	37		$Mn(OH)^{2+} + H_2O \rightleftharpoons Mn(OH)_2^+ + H^+$	$1\cdot10^{-5}$	$2\cdot10^{5}$		B	$2\cdot10^{10}$		B	"
*	38		$Mn^{2+} + HSO_3^- \rightleftharpoons MnHSO_3^+$	$3\cdot10^{4}$	$3.1\cdot10^{7}$		C	$1.033\cdot10^{3}$		C	"
*	39		$Cu^{2+} + OH \rightleftharpoons CuOH^{2+}$	$1.17\cdot10^{4}$	$3.5\cdot10^{8}$		D	$3\cdot10^{4}$		E	
	40		$HO_3 \rightleftharpoons H^+ + O_3^-$	$5 \cdot10^{-9}$	330		F	$5.2\cdot10^{10}$		F	sink for O_3^- (see R31/32)
*	41		$HOONO \rightleftharpoons H^+ + OONO^-$	$1\cdot10^{-6}$	$5\cdot10^{4}$		G	$5\cdot10^{10}$		(E)	HOONO new added (see reaction 81)
	42		$CHOHSO_3^- \rightleftharpoons CHOSO_3^{2-} + H^+$	$1.34 \cdot10^{-6}$	$5.9\cdot10^{4}$		H	$4.4\cdot10^{10}$		H	link between acid/anion
	43		$SO_5O_2H \rightleftharpoons SO_5O_2^- + H^+$	$1.6 \cdot10^{-5}$	$7.5\cdot10^{5}$			$5\cdot10^{10}$		(E)	"

*	44		$H_2C_2O_4 \rightleftharpoons H^+ + HC_2O_4^-$	$6.4 \cdot 10^{-2}$	$3.2 \cdot 10^9$			$5 \cdot 10^{10}$	(E)	consideration of C_2-difunctional compounds
	45		$HC_2O_4^- \rightleftharpoons H^+ + C_2O_4^{2-}$	$5.25 \cdot 10^{-5}$	$2.6 \cdot 10^6$			$5 \cdot 10^{10}$	(E)	"
	46		$CH(OH)_2COOH \rightleftharpoons H^+ + CH(OH)_2COO^-$	$3.16 \cdot 10^{-4}$	$6.32 \cdot 10^6$		J	$2 \cdot 10^{10}$	J	"
	47		$CHOCHO + H_2O \rightleftharpoons (CH(OH)_2)_2$	$3.9 \cdot 10^3$	21.5		K	$5.5 \cdot 10^{-3}$	K	"
	48		$[Fe(C_2O_4)]^+ \rightleftharpoons [Fe]^{3+} + C_2O_4^{2-}$	$2.9 \cdot 10^9$	$3 \cdot 10^{-3}$		L	$7.5 \cdot 10^6$		"
	49		$[Fe(C_2O_4)_2]^- \rightleftharpoons [Fe(C_2O_4)]^+ + C_2O_4^{2-}$	$6.3 \cdot 10^6$	$3 \cdot 10^{-3}$		(E)	$1.89 \cdot 10^4$		"
*	50		$[Fe(C_2O_4)_3]^{3-} \rightleftharpoons [Fe(C_2O_4)_2]^- + C_2O_4^{2-}$	$3.8 \cdot 10^4$	$3 \cdot 10^{-3}$		(E)	38		"
	51		$SO_4^- + Cl^- \rightleftharpoons SO_4^{2-} + Cl$	1.2	$2.52 \cdot 10^8$		M	$2.1 \cdot 10^8$	M	dat for back reaction available
	52		$NO_3 + Cl^- \rightleftharpoons NO_3^- + Cl$	3.4	$3.4 \cdot 10^8$		N	$1 \cdot 10^8$	N	"
*	53		$Cl^- + Fe^{3+} \rightleftharpoons FeCl^{2+}$	1.39	$3 \cdot 10^3$		O	2160		
*	54		**$CH_3C(O)OOH$** $\rightleftharpoons CH_3C(O)OO^- + H^+$	$6.3 \cdot 10^{-9}$	315		P	$5 \cdot 10^{10}$	(E)	sink for the anion (see R255)
	55		$CH_3CO + H_2O \rightleftharpoons CH_3C(OH)_2$	367	$1.1 \cdot 10^7$		Q	$3 \cdot 10^4$		hydration of acetyl radical analogous to acetaldehyde
*	56		$2\ Br^- + CO_3^- \rightleftharpoons Br_2^- + CO_3^{2-}$	0.34	$3.4 \cdot 10^4$		R	$1.1 \cdot 10^5$	R	
	57		$ACO_3 \rightleftharpoons O_2CH_2COO^- + H^+$	$1.75 \cdot 10^{-5}$	$8.75 \cdot 10^5$	**-46**	S	$5 \cdot 10^{10}$	S	sink for the anion (R265); additional to recombinations 250-253

[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; Boyce and Hoffmann, 1996, [r] Buxton *et al.*, 1998; [s] Merényi and Lind, 1994; [t] Jayson *et al.*, 1973; [u] Grigor'ev et al., 1987; [v] Zehavi and Rabani, 1972; [w] Kläning and Wolff, 1985; [x] Fornier de Violet, 1981; [y] Wells and Davies, 1967, [z] Jacobsen *et al.*, 1997b; [A] Rosseinsky, 1963; [B] v. Piechowski *et al.*, 1993; [C] Berglund et al., 1993; [D] Buxton *et al.*, 1988; [E] Meyerstein, 1971; [F] Bühler et al., 1984; [G] Wagner *et al.*, 1980; [H] Barlow *et al.*, 1997b; [I] Sedlak and Hoigne, 1993; [J] Buxton *et al.*, 1997; [K] Betterton and Hoffmann, 1988a; [L] Moorhead and Sutin, 1967; [M] Buxton *et al.*, 1999b; [N] Buxton *et al.*, 1999c; [O] Martell and Sillen; [P] Schuchmann and v. Sonntag, 1988; [R]Lilie *et al.*, 1978; [S] estimated equal as acetic acid

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